



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 6, 2026 – 03:26 pm BST

PDB ID : 9RTD / pdb_00009rtd
Title : Crystal structure of DNA aptamer C8N5t in complex with Plasmodium falciparum lactate dehydrogenase
Authors : Tars, K.
Deposited on : 2025-07-02
Resolution : 2.10 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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

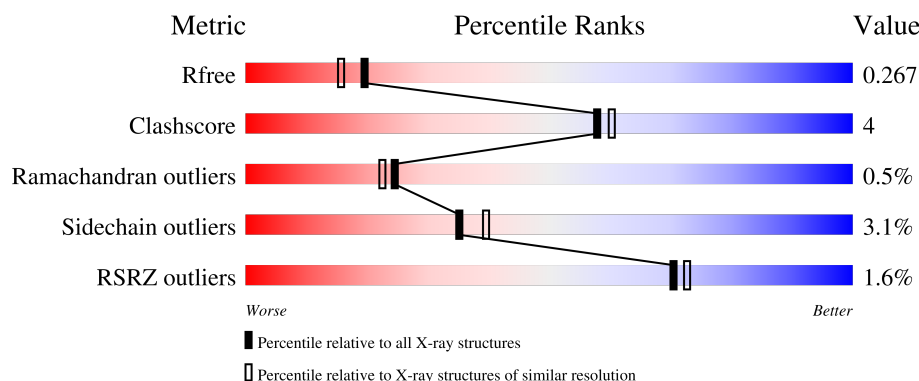
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	A	329	
1	B	329	
1	C	329	
1	D	329	
2	G	40	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10134 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 protein called L-lactate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	306	Total	C	N	O	S	0	0	0
			2313	1473	395	432	13			
1	B	310	Total	C	N	O	S	0	0	0
			2347	1497	401	436	13			
1	C	306	Total	C	N	O	S	0	0	0
			2320	1479	396	432	13			
1	D	307	Total	C	N	O	S	0	0	0
			2327	1484	397	433	13			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	MET	-	initiating methionine	UNP Q27743
A	-11	ALA	-	expression tag	UNP Q27743
A	-10	HIS	-	expression tag	UNP Q27743
A	-9	HIS	-	expression tag	UNP Q27743
A	-8	HIS	-	expression tag	UNP Q27743
A	-7	HIS	-	expression tag	UNP Q27743
A	-6	HIS	-	expression tag	UNP Q27743
A	-5	HIS	-	expression tag	UNP Q27743
A	-4	GLU	-	expression tag	UNP Q27743
A	-3	ASN	-	expression tag	UNP Q27743
A	-2	LEU	-	expression tag	UNP Q27743
A	-1	TYR	-	expression tag	UNP Q27743
A	0	PHE	-	expression tag	UNP Q27743
A	1	GLN	-	expression tag	UNP Q27743
B	-12	MET	-	initiating methionine	UNP Q27743
B	-11	ALA	-	expression tag	UNP Q27743
B	-10	HIS	-	expression tag	UNP Q27743
B	-9	HIS	-	expression tag	UNP Q27743
B	-8	HIS	-	expression tag	UNP Q27743
B	-7	HIS	-	expression tag	UNP Q27743
B	-6	HIS	-	expression tag	UNP Q27743

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	HIS	-	expression tag	UNP Q27743
B	-4	GLU	-	expression tag	UNP Q27743
B	-3	ASN	-	expression tag	UNP Q27743
B	-2	LEU	-	expression tag	UNP Q27743
B	-1	TYR	-	expression tag	UNP Q27743
B	0	PHE	-	expression tag	UNP Q27743
B	1	GLN	-	expression tag	UNP Q27743
C	-12	MET	-	initiating methionine	UNP Q27743
C	-11	ALA	-	expression tag	UNP Q27743
C	-10	HIS	-	expression tag	UNP Q27743
C	-9	HIS	-	expression tag	UNP Q27743
C	-8	HIS	-	expression tag	UNP Q27743
C	-7	HIS	-	expression tag	UNP Q27743
C	-6	HIS	-	expression tag	UNP Q27743
C	-5	HIS	-	expression tag	UNP Q27743
C	-4	GLU	-	expression tag	UNP Q27743
C	-3	ASN	-	expression tag	UNP Q27743
C	-2	LEU	-	expression tag	UNP Q27743
C	-1	TYR	-	expression tag	UNP Q27743
C	0	PHE	-	expression tag	UNP Q27743
C	1	GLN	-	expression tag	UNP Q27743
D	-12	MET	-	initiating methionine	UNP Q27743
D	-11	ALA	-	expression tag	UNP Q27743
D	-10	HIS	-	expression tag	UNP Q27743
D	-9	HIS	-	expression tag	UNP Q27743
D	-8	HIS	-	expression tag	UNP Q27743
D	-7	HIS	-	expression tag	UNP Q27743
D	-6	HIS	-	expression tag	UNP Q27743
D	-5	HIS	-	expression tag	UNP Q27743
D	-4	GLU	-	expression tag	UNP Q27743
D	-3	ASN	-	expression tag	UNP Q27743
D	-2	LEU	-	expression tag	UNP Q27743
D	-1	TYR	-	expression tag	UNP Q27743
D	0	PHE	-	expression tag	UNP Q27743
D	1	GLN	-	expression tag	UNP Q27743

- Molecule 2 is a DNA chain called DNA (32-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	32	Total	C	N	O	P	0	0	0
			661	315	120	194	32			

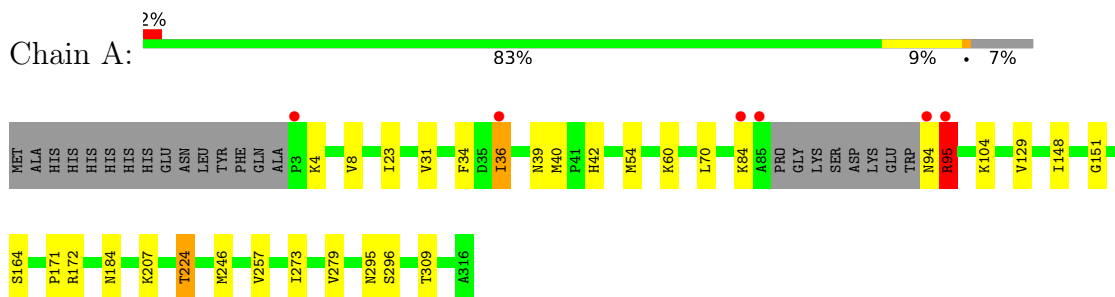
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	37	Total 37	O 37	0	0
3	B	39	Total 39	O 39	0	0
3	C	38	Total 38	O 38	0	0
3	D	44	Total 44	O 44	0	0
3	G	8	Total 8	O 8	0	0

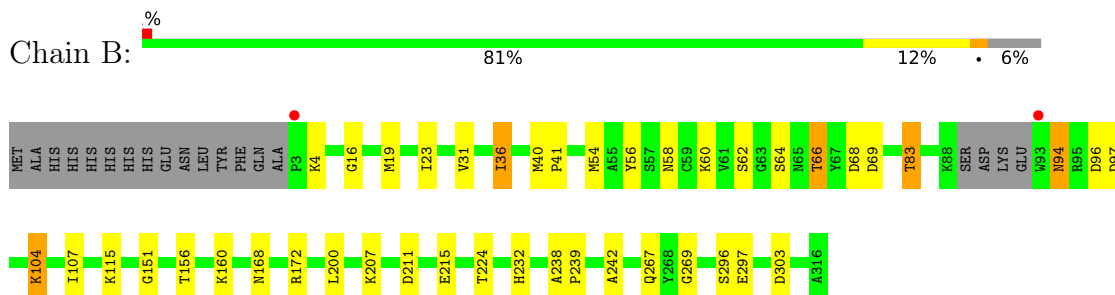
3 Residue-property plots [i](#)

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.

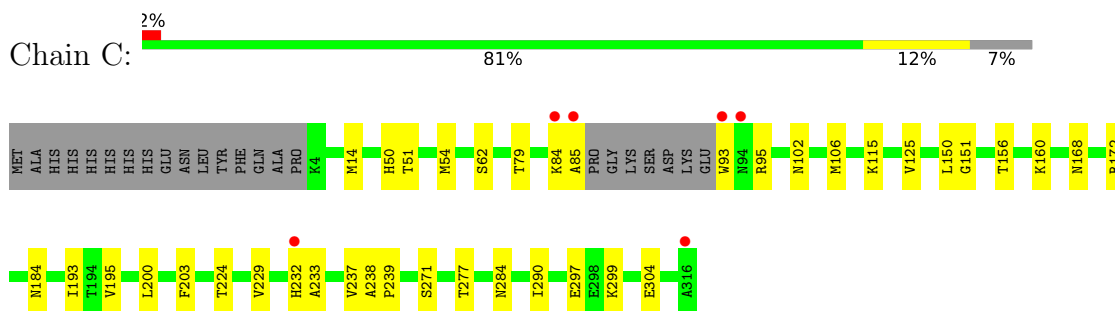
- Molecule 1: L-lactate dehydrogenase



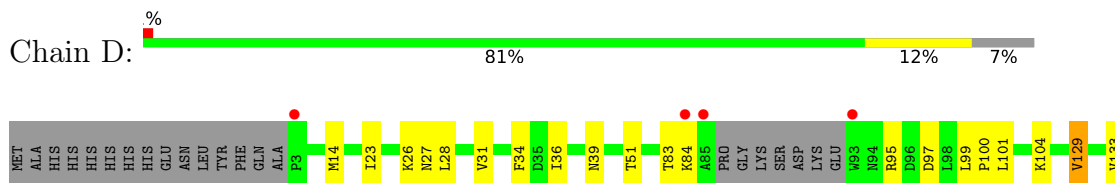
- Molecule 1: L-lactate dehydrogenase



- Molecule 1: L-lactate dehydrogenase

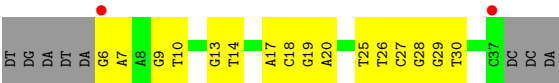


- Molecule 1: L-lactate dehydrogenase





• Molecule 2: DNA (32-MER)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	92.11Å 105.57Å 158.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	87.95 – 2.10 87.95 – 2.10	Depositor EDS
% Data completeness (in resolution range)	59.8 (87.95-2.10) 59.8 (87.95-2.10)	Depositor EDS
R_{merge}	0.35	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 1.94Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.202 , 0.267 0.209 , 0.267	Depositor DCC
R_{free} test set	2786 reflections (2.44%)	wwPDB-VP
Wilson B-factor (Å ²)	20.1	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 25.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10134	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.76% 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

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	A	0.61	0/2346	1.16	5/3174 (0.2%)
1	B	0.63	0/2383	1.18	7/3225 (0.2%)
1	C	0.59	0/2354	1.15	5/3186 (0.2%)
1	D	0.62	0/2362	1.14	2/3197 (0.1%)
2	G	0.43	0/741	1.16	3/1143 (0.3%)
All	All	0.60	0/10186	1.16	22/13925 (0.2%)

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
1	C	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	184	ASN	CB-CA-C	-10.21	91.74	110.63
1	B	168	ASN	CB-CA-C	-9.17	98.72	112.11
1	C	284	ASN	CB-CA-C	-6.60	98.62	110.37
1	A	60	LYS	CB-CA-C	-6.23	99.92	109.89
1	B	54	MET	CG-SD-CE	6.21	114.55	100.90
1	C	168	ASN	CB-CA-C	6.18	122.71	110.42
2	G	17	DA	O3'-P-O5'	-6.10	94.85	104.00
1	C	299	LYS	N-CA-CB	6.07	119.05	110.12
1	A	184	ASN	CB-CA-C	-5.80	101.16	110.79
1	B	83	THR	N-CA-CB	-5.78	103.35	110.98
1	D	304	GLU	CB-CA-C	-5.74	101.26	110.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	68	ASP	CA-CB-CG	5.71	118.31	112.60
1	D	168	ASN	CB-CA-C	-5.52	104.05	111.89
1	B	66	THR	OG1-CB-CG2	5.46	120.22	109.30
1	A	4	LYS	N-CA-CB	-5.42	102.96	110.38
1	B	303	ASP	CB-CA-C	5.40	119.76	110.79
1	A	60	LYS	N-CA-CB	5.39	117.88	109.85
2	G	9	DG	O3'-P-O5'	-5.27	96.09	104.00
1	C	304	GLU	CB-CG-CD	5.20	121.44	112.60
1	A	224	THR	CA-CB-OG1	-5.03	102.06	109.60
2	G	29	DG	O3'-P-O5'	-5.01	96.48	104.00
1	B	96	ASP	CA-CB-CG	5.00	117.60	112.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	172	ARG	Sidechain
1	D	83	THR	Peptide

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	A	2313	0	2402	19	0
1	B	2347	0	2435	24	0
1	C	2320	0	2404	16	0
1	D	2327	0	2412	27	0
2	G	661	0	363	15	0
3	A	37	0	0	0	0
3	B	39	0	0	1	0
3	C	38	0	0	1	0
3	D	44	0	0	0	0
3	G	8	0	0	2	0
All	All	10134	0	10016	89	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 4.

All (89) 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)
1:B:83:THR:HG23	2:G:13:DG:N7	1.81	0.96
1:C:232:HIS:HB2	3:C:437:HOH:O	1.90	0.71
1:D:299:LYS:O	1:D:299:LYS:HD3	1.95	0.66
1:D:172:ARG:O	1:D:172:ARG:HG3	1.97	0.64
2:G:13:DG:H2''	2:G:14:DT:OP2	1.99	0.64
1:B:83:THR:HG21	3:G:102:HOH:O	2.00	0.60
2:G:30:DT:H2'	2:G:30:DT:O2	2.01	0.60
1:D:273:ILE:HD11	1:D:309:THR:HG22	1.85	0.58
1:D:299:LYS:HD2	1:D:303:ASP:OD2	2.05	0.57
2:G:10:DT:H5''	2:G:10:DT:H6	1.70	0.57
1:D:23:ILE:HG21	1:D:31:VAL:HG22	1.88	0.56
1:D:236:TYR:C	1:D:239:PRO:HD2	2.32	0.55
1:A:295:ASN:OD1	1:A:295:ASN:C	2.47	0.55
2:G:6:DG:H2''	2:G:7:DA:OP2	2.07	0.55
1:A:54:MET:HE3	1:B:242:ALA:HB2	1.89	0.54
1:B:23:ILE:HG21	1:B:31:VAL:HG22	1.90	0.54
1:C:238:ALA:HB3	1:C:239:PRO:HD3	1.89	0.54
1:D:95:ARG:HH11	1:D:95:ARG:HG3	1.72	0.53
1:B:16:GLY:HA2	1:B:19:MET:HE3	1.90	0.53
1:B:4:LYS:NZ	1:B:58:ASN:O	2.41	0.53
1:B:211:ASP:O	1:B:215:GLU:HG2	2.08	0.53
1:C:237:VAL:HG12	1:D:51:THR:HG21	1.91	0.53
1:A:23:ILE:HG21	1:A:31:VAL:HG22	1.91	0.52
1:D:192:TYR:CE1	1:D:292:LEU:HD22	2.44	0.52
1:B:83:THR:CG2	3:G:102:HOH:O	2.56	0.52
1:A:36:ILE:CD1	2:G:20:DA:O4'	2.58	0.51
1:D:299:LYS:HD3	1:D:299:LYS:C	2.36	0.50
1:C:84:LYS:O	1:C:85:ALA:C	2.54	0.50
1:A:36:ILE:HD11	2:G:20:DA:O4'	2.12	0.50
1:A:23:ILE:HG21	1:A:31:VAL:CG2	2.42	0.50
1:A:36:ILE:HD11	2:G:20:DA:H5'	1.94	0.49
1:C:156:THR:O	1:C:160:LYS:HG3	2.12	0.49
1:A:39:ASN:HA	1:A:42:HIS:HD2	1.78	0.49
1:C:193:ILE:HG21	1:C:200:LEU:HD22	1.95	0.49
1:C:195:VAL:HB	1:C:203:PHE:CE1	2.48	0.48
1:C:229:VAL:HA	1:C:233:ALA:O	2.14	0.47
1:A:95:ARG:HH11	1:A:95:ARG:HB3	1.79	0.47
1:D:97:ASP:O	1:D:100:PRO:HD2	2.14	0.47
1:B:156:THR:HB	1:B:160:LYS:HE3	1.97	0.47
1:D:238:ALA:N	1:D:239:PRO:CD	2.78	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:101:LEU:O	1:D:104:LYS:HB2	2.15	0.46
1:B:36:ILE:CD1	1:B:36:ILE:H	2.28	0.46
1:B:16:GLY:HA2	1:B:19:MET:CE	2.46	0.46
1:C:102:ASN:O	1:C:106:MET:HG2	2.16	0.46
1:B:64:SER:OG	1:B:69:ASP:OD2	2.17	0.45
1:B:232:HIS:CD2	3:B:407:HOH:O	2.68	0.45
1:C:51:THR:HA	1:C:54:MET:HE2	1.99	0.45
1:B:23:ILE:HG21	1:B:31:VAL:CG2	2.46	0.45
1:A:273:ILE:HD11	1:A:309:THR:HG22	1.98	0.45
1:D:270:HIS:NE2	1:D:303:ASP:OD1	2.48	0.45
1:B:238:ALA:HB3	1:B:239:PRO:HD3	1.97	0.45
2:G:27:DC:H2''	2:G:28:DG:C2	2.52	0.45
1:A:148:ILE:HD12	1:A:246:MET:HE3	1.99	0.45
1:C:277:THR:OG1	1:C:290:ILE:O	2.34	0.45
1:B:267:GLN:C	1:B:269:GLY:H	2.25	0.44
1:B:36:ILE:HD13	1:B:36:ILE:N	2.32	0.44
1:B:36:ILE:H	1:B:36:ILE:HD13	1.81	0.44
1:D:238:ALA:HB3	1:D:239:PRO:HD3	2.00	0.44
1:D:311:ARG:HG2	1:D:311:ARG:HH11	1.83	0.44
1:A:257:VAL:HA	1:A:279:VAL:O	2.18	0.44
1:B:40:MET:N	1:B:41:PRO:HD2	2.33	0.44
1:B:94:ASN:O	1:B:97:ASP:HB2	2.18	0.44
1:C:14:MET:CE	1:D:14:MET:HE1	2.47	0.44
1:D:99:LEU:N	1:D:100:PRO:HD2	2.33	0.44
2:G:25:DT:H2''	2:G:26:DT:OP2	2.17	0.43
1:A:36:ILE:HD13	2:G:20:DA:C4	2.54	0.43
1:A:164:SER:CB	1:A:171:PRO:HA	2.49	0.43
1:A:172:ARG:O	1:A:172:ARG:HG2	2.18	0.43
1:D:231:LEU:O	1:D:232:HIS:HB2	2.19	0.43
1:D:95:ARG:HH11	1:D:95:ARG:CG	2.32	0.42
1:D:28:LEU:HD23	1:D:28:LEU:HA	1.84	0.42
1:A:172:ARG:HD3	1:B:56:TYR:CD2	2.55	0.42
2:G:18:DC:H2''	2:G:19:DG:O5'	2.20	0.42
2:G:6:DG:C8	2:G:6:DG:OP2	2.73	0.41
1:C:95:ARG:HG3	1:C:95:ARG:HH11	1.85	0.41
1:A:8:VAL:HG11	1:A:70:LEU:HD23	2.03	0.41
1:B:172:ARG:O	1:B:172:ARG:HG2	2.20	0.41
1:D:23:ILE:HG21	1:D:31:VAL:CG2	2.50	0.41
1:C:115:LYS:O	1:C:115:LYS:HG3	2.20	0.41
1:D:129:VAL:O	1:D:133:VAL:HG12	2.21	0.41
1:A:40:MET:HG3	2:G:19:DG:C2	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:148:ILE:HD12	1:D:246:MET:HE3	2.01	0.41
1:B:104:LYS:HA	1:B:107:ILE:HD12	2.03	0.41
1:A:34:PHE:CD1	1:A:34:PHE:C	2.99	0.40
1:C:50:HIS:CE1	1:D:158:ARG:HG2	2.57	0.40
1:C:125:VAL:HG13	1:C:150:LEU:HD23	2.04	0.40
1:D:26:LYS:O	1:D:27:ASN:C	2.63	0.40
1:D:34:PHE:CD2	1:D:34:PHE:C	2.99	0.40
1:B:83:THR:CG2	2:G:13:DG:N7	2.69	0.40

There are no symmetry-related clashes.

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	
1	A	302/329 (92%)	289 (96%)	11 (4%)	2 (1%)	18	15
1	B	306/329 (93%)	297 (97%)	8 (3%)	1 (0%)	36	36
1	C	302/329 (92%)	291 (96%)	10 (3%)	1 (0%)	36	36
1	D	303/329 (92%)	292 (96%)	9 (3%)	2 (1%)	18	15
All	All	1213/1316 (92%)	1169 (96%)	38 (3%)	6 (0%)	24	22

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	95	ARG
1	D	151	GLY
1	C	151	GLY
1	A	151	GLY
1	D	39	ASN
1	B	151	GLY

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	
1	A	255/275 (93%)	246 (96%)	9 (4%)	32	35
1	B	258/275 (94%)	246 (95%)	12 (5%)	23	24
1	C	255/275 (93%)	249 (98%)	6 (2%)	43	49
1	D	256/275 (93%)	251 (98%)	5 (2%)	48	56
All	All	1024/1100 (93%)	992 (97%)	32 (3%)	35	39

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	ILE
1	A	84	LYS
1	A	94	ASN
1	A	95	ARG
1	A	104	LYS
1	A	129	VAL
1	A	207	LYS
1	A	224	THR
1	A	296	SER
1	B	36	ILE
1	B	60	LYS
1	B	62	SER
1	B	66	THR
1	B	94	ASN
1	B	104	LYS
1	B	115	LYS
1	B	200	LEU
1	B	207	LYS
1	B	224	THR
1	B	296	SER
1	B	297	GLU
1	C	62	SER
1	C	79	THR
1	C	93	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	224	THR
1	C	271	SER
1	C	297	GLU
1	D	36	ILE
1	D	84	LYS
1	D	129	VAL
1	D	171	PRO
1	D	207	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	116	ASN
1	A	165	GLN
1	A	184	ASN
1	A	223	ASN
1	A	284	ASN
1	B	25	GLN
1	B	94	ASN
1	B	201	GLN
1	B	223	ASN
1	C	165	GLN
1	C	201	GLN
1	C	206	ASN
1	C	223	ASN
1	C	284	ASN
1	D	25	GLN
1	D	103	ASN
1	D	116	ASN
1	D	165	GLN
1	D	223	ASN
1	D	284	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	A	306/329 (93%)	-0.06	6 (1%) 65 67	9, 18, 35, 61	0
1	B	310/329 (94%)	-0.15	2 (0%) 85 87	8, 17, 32, 55	0
1	C	306/329 (93%)	-0.00	6 (1%) 65 67	11, 20, 34, 104	0
1	D	307/329 (93%)	-0.03	4 (1%) 75 77	10, 18, 34, 93	0
2	G	32/40 (80%)	0.32	2 (6%) 26 27	24, 38, 85, 103	0
All	All	1261/1356 (92%)	-0.05	20 (1%) 70 73	8, 19, 37, 104	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	93	TRP	6.8
1	D	93	TRP	6.0
1	A	85	ALA	5.9
1	A	3	PRO	5.5
1	A	84	LYS	5.0
1	D	3	PRO	4.5
1	D	85	ALA	3.6
1	A	95	ARG	3.4
1	C	85	ALA	3.4
1	D	84	LYS	3.3
1	C	232	HIS	3.2
2	G	6	DG	2.9
1	A	36	ILE	2.8
1	C	316	ALA	2.7
1	B	3	PRO	2.7
2	G	37	DC	2.5
1	A	94	ASN	2.4
1	C	94	ASN	2.2
1	C	84	LYS	2.2
1	B	93	TRP	2.1

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.