



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:36 AM UTC

PDB ID : 1YSA / pdb_00001ysa
Title : THE GCN4 BASIC REGION LEUCINE ZIPPER BINDS DNA AS A DIMER OF UNINTERRUPTED ALPHA HELICES: CRYSTAL STRUCTURE OF THE PROTEIN-DNA COMPLEX
Authors : Ellenberger, T.E.; Brandl, C.J.; Struhl, K.; Harrison, S.C.
Deposited on : 1993-08-09
Resolution : 2.90 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

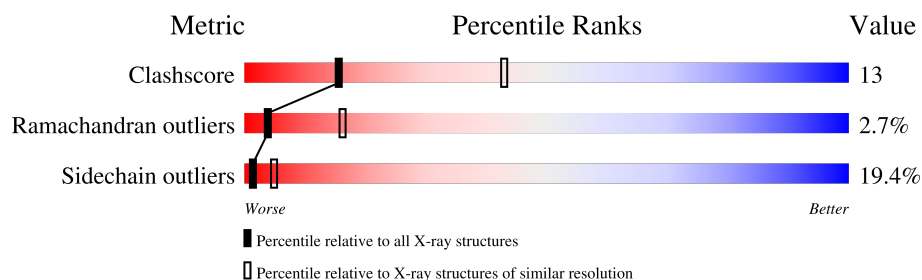
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	20	15% 45% 40%
2	B	20	10% 35% 55%
3	C	58	34% 40% 21% ••
3	D	58	24% 52% 19% ••

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 1772 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(*TP*TP*CP*CP*TP*AP*TP*GP*AP*CP*TP*CP*AP*TP*CP*CP*A P*GP*TP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	20	Total	C	N	O	P	0	0	0
			399	194	64	122	19			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	20	Total	C	N	O	P	0	0	0
			415	198	84	114	19			

- Molecule 3 is a protein called PROTEIN (GCN4).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	57	Total	C	N	O	S	0	0	0
			472	288	99	84	1			
3	D	57	Total	C	N	O	S	0	0	0
			469	287	96	84	2			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	4	Total	O	0	0
			4	4		
4	B	2	Total	O	0	0
			2	2		
4	C	4	Total	O	0	0
			4	4		
4	D	7	Total	O	0	0
			7	7		

3 Residue-property plots

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. 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. 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.

Note EDS was not executed.

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

Chain A: 

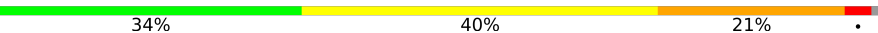


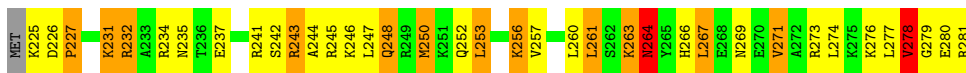
- Molecule 2: DNA (5'-D(*AP*AP*AP*CP*TP*GP*GP*AP*TP*GP*AP*GP*TP*CP*AP*TP*A P*GP*GP*A)-3')

Chain B: 

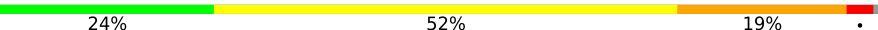


- Molecule 3: PROTEIN (GCN4)

Chain C: 



- Molecule 3: PROTEIN (GCN4)

Chain D: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	49.13Å 88.54Å 59.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.90)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.230 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1772	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

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	1.16	0/444	2.48	41/682 (6.0%)
2	B	1.43	7/468 (1.5%)	2.64	47/722 (6.5%)
3	C	1.52	4/474 (0.8%)	2.67	36/627 (5.7%)
3	D	1.45	4/471 (0.8%)	2.68	42/623 (6.7%)
All	All	1.40	15/1857 (0.8%)	2.62	166/2654 (6.3%)

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
2	B	0	1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	278	VAL	CA-CB	9.50	1.67	1.54
2	B	24	DC	O3'-P	6.92	1.71	1.61
3	D	266	HIS	CD2-NE2	-6.82	1.30	1.37
3	C	278	VAL	CA-C	6.75	1.61	1.52
2	B	32	DG	O3'-P	-6.45	1.51	1.61
3	D	279	GLY	CA-C	5.90	1.58	1.51
2	B	39	DG	P-O5'	5.69	1.71	1.60
2	B	39	DG	C5'-C4'	5.68	1.63	1.52
2	B	25	DT	O3'-P	5.54	1.69	1.61
3	D	262	SER	CA-CB	-5.25	1.45	1.53
2	B	35	DA	O3'-P	5.21	1.69	1.61
2	B	26	DG	C5'-C4'	-5.17	1.42	1.52
3	D	266	HIS	CG-ND1	-5.17	1.32	1.38
3	C	266	HIS	CG-ND1	-5.08	1.32	1.38
3	C	266	HIS	CD2-NE2	-5.03	1.32	1.37

All (166) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	9	DA	O3'-P-O5'	-15.14	81.29	104.00
2	B	34	DC	P-O3'-C3'	14.21	141.52	120.20
2	B	22	DA	P-O3'-C3'	12.40	138.80	120.20
3	C	264	ASN	OD1-CG-ND2	-12.33	110.27	122.60
3	D	235	ASN	OD1-CG-ND2	-11.78	110.82	122.60
3	C	248	GLN	OE1-CD-NE2	-11.15	111.45	122.60
2	B	29	DT	P-O5'-C5'	-10.52	104.22	120.00
2	B	32	DG	O3'-P-O5'	-10.37	88.44	104.00
2	B	34	DC	C4'-C3'-O3'	10.33	125.50	110.00
3	D	262	SER	CA-CB-OG	-10.24	90.63	111.10
2	B	21	DA	O3'-P-O5'	-9.94	89.09	104.00
3	D	264	ASN	OD1-CG-ND2	-9.76	112.84	122.60
3	C	271	VAL	N-CA-C	-9.75	101.25	110.42
3	D	255	ASP	N-CA-C	-9.71	100.65	111.14
2	B	34	DC	C2'-C3'-O3'	-9.68	96.99	111.50
3	C	278	VAL	O-C-N	-9.51	110.69	122.57
1	A	4	DC	P-O3'-C3'	9.25	134.07	120.20
2	B	39	DG	C5'-C4'-C3'	-9.21	101.08	114.90
2	B	21	DA	P-O3'-C3'	9.03	133.74	120.20
3	C	244	ALA	N-CA-C	8.95	122.16	111.33
3	C	263	LYS	CA-C-O	-8.82	111.81	120.90
1	A	19	DT	O3'-P-O5'	-8.71	90.94	104.00
2	B	39	DG	C5'-C4'-O4'	8.67	122.41	109.40
3	D	238	ALA	CA-C-O	-8.66	111.55	121.07
1	A	16	DC	O3'-P-O5'	-8.59	91.12	104.00
2	B	30	DG	C4'-C3'-O3'	-8.57	97.14	110.00
2	B	31	DA	P-O3'-C3'	8.38	132.77	120.20
1	A	12	DC	O3'-P-O5'	-8.31	91.54	104.00
3	D	243	ARG	O-C-N	-8.12	112.89	122.15
3	D	225	LYS	N-CA-C	8.02	127.88	110.80
3	D	279	GLY	N-CA-C	7.98	121.67	111.37
2	B	38	DG	P-O3'-C3'	7.98	132.16	120.20
1	A	19	DT	O4'-C1'-C2'	-7.95	94.48	106.40
3	C	248	GLN	CG-CD-NE2	7.91	128.26	116.40
2	B	22	DA	P-O5'-C5'	-7.78	108.33	120.00
2	B	38	DG	O4'-C1'-C2'	-7.74	94.79	106.40
2	B	30	DG	P-O3'-C3'	7.70	131.75	120.20
1	A	1	DT	P-O3'-C3'	-7.69	108.67	120.20
3	D	239	ALA	CA-C-O	-7.66	112.36	120.63
3	C	263	LYS	N-CA-C	-7.65	102.54	111.03
1	A	15	DC	O4'-C1'-C2'	-7.64	94.93	106.40
3	C	252	GLN	OE1-CD-NE2	-7.62	114.98	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	8	DG	O5'-C5'-C4'	7.56	122.14	110.80
3	D	263	LYS	N-CA-C	-7.55	102.74	110.97
2	B	25	DT	C6-N1-C1'	7.46	130.54	119.35
3	D	228	ALA	CA-C-O	-7.29	111.86	120.10
3	D	243	ARG	CB-CG-CD	7.27	128.01	111.30
3	D	235	ASN	CB-CG-ND2	7.26	127.30	116.40
3	C	269	ASN	OD1-CG-ND2	-7.21	115.39	122.60
2	B	40	DA	O4'-C1'-C2'	-7.17	95.65	106.40
1	A	15	DC	P-O3'-C3'	7.15	130.92	120.20
3	D	244	ALA	O-C-N	-7.14	114.72	122.07
3	D	249	ARG	N-CA-C	-7.14	103.58	111.36
1	A	4	DC	C4'-C3'-C2'	-7.09	91.77	102.40
1	A	2	DT	O4'-C1'-N1	-7.08	97.78	108.40
3	C	271	VAL	CA-C-O	-7.08	112.97	121.18
2	B	29	DT	O5'-C5'-C4'	7.05	121.38	110.80
3	C	234	ARG	N-CA-C	7.05	120.36	111.69
1	A	9	DA	C2'-C3'-O3'	-7.04	100.93	111.50
2	B	39	DG	O5'-C5'-C4'	7.04	121.36	110.80
1	A	3	DC	O5'-C5'-C4'	7.02	121.33	110.80
3	C	242	SER	N-CA-C	7.02	118.93	111.28
3	C	235	ASN	OD1-CG-ND2	-6.96	115.64	122.60
2	B	24	DC	C3'-C2'-C1'	6.94	112.02	101.60
3	D	252	GLN	OE1-CD-NE2	-6.93	115.67	122.60
1	A	1	DT	C2'-C3'-O3'	-6.92	101.12	111.50
3	D	248	GLN	OE1-CD-NE2	-6.90	115.70	122.60
2	B	35	DA	O5'-C5'-C4'	6.86	121.09	110.80
1	A	18	DG	O5'-C5'-C4'	6.85	121.08	110.80
3	C	242	SER	CB-CA-C	-6.81	99.49	110.79
1	A	15	DC	C4'-C3'-O3'	-6.81	99.79	110.00
2	B	34	DC	C3'-C2'-C1'	6.80	111.80	101.60
2	B	23	DA	C1'-O4'-C4'	-6.78	99.53	109.70
2	B	27	DG	O5'-C5'-C4'	6.74	120.91	110.80
1	A	2	DT	O4'-C1'-C2'	-6.69	96.36	106.40
1	A	8	DG	N9-C1'-C2'	-6.64	103.53	113.50
1	A	12	DC	C5'-C4'-C3'	-6.61	104.98	114.90
3	D	280	GLU	N-CA-C	6.61	129.51	111.00
1	A	11	DT	O4'-C1'-C2'	-6.60	96.50	106.40
2	B	26	DG	O4'-C4'-C3'	6.54	115.21	105.40
1	A	6	DA	O3'-P-O5'	-6.47	94.29	104.00
1	A	16	DC	P-O3'-C3'	6.47	129.91	120.20
2	B	25	DT	P-O5'-C5'	6.45	129.68	120.00
3	C	243	ARG	N-CA-C	-6.41	104.22	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	248	GLN	O-C-N	-6.40	114.40	122.27
3	D	232	ARG	O-C-N	-6.37	115.15	122.03
1	A	14	DT	C3'-C2'-C1'	6.36	111.14	101.60
2	B	25	DT	C5'-C4'-C3'	-6.34	105.40	114.90
3	C	264	ASN	CB-CG-ND2	6.30	125.85	116.40
1	A	4	DC	C3'-C2'-C1'	6.28	111.01	101.60
3	C	247	LEU	CB-CA-C	-6.26	101.05	110.88
3	D	243	ARG	CA-CB-CG	-6.25	101.59	114.10
3	D	261	LEU	O-C-N	6.20	128.69	122.12
3	D	263	LYS	N-CA-CB	6.17	118.92	109.91
2	B	24	DC	C4'-C3'-O3'	6.13	119.20	110.00
1	A	4	DC	O4'-C4'-C3'	6.13	114.59	105.40
3	C	246	LYS	CA-CB-CG	-6.07	101.96	114.10
2	B	30	DG	C5'-C4'-C3'	-6.04	105.84	114.90
1	A	12	DC	P-O3'-C3'	6.03	129.25	120.20
1	A	8	DG	O4'-C1'-N9	6.03	117.44	108.40
3	D	265	TYR	CB-CA-C	-5.96	100.89	110.79
3	D	256	LYS	O-C-N	-5.92	115.85	122.12
3	D	263	LYS	CB-CA-C	-5.91	101.85	110.96
1	A	5	DT	O3'-P-O5'	-5.90	95.15	104.00
1	A	8	DG	O3'-P-O5'	-5.88	95.18	104.00
1	A	10	DC	P-O3'-C3'	5.87	129.00	120.20
1	A	5	DT	P-O3'-C3'	5.86	128.99	120.20
2	B	27	DG	O4'-C1'-C2'	-5.84	97.64	106.40
1	A	12	DC	P-O5'-C5'	-5.82	111.26	120.00
3	C	267	LEU	CA-C-O	-5.82	114.71	120.82
3	D	266	HIS	CB-CG-CD2	-5.79	123.68	131.20
2	B	34	DC	O3'-P-O5'	-5.77	95.35	104.00
3	D	255	ASP	CA-CB-CG	5.76	118.36	112.60
2	B	39	DG	P-O5'-C5'	5.74	128.60	120.00
3	C	226	ASP	CA-CB-CG	5.74	118.33	112.60
3	C	263	LYS	CG-CD-CE	5.71	124.44	111.30
2	B	23	DA	C5'-C4'-O4'	-5.70	100.84	109.40
1	A	1	DT	C5'-C4'-C3'	-5.67	106.39	114.90
2	B	25	DT	C4-C5-C7	-5.67	113.90	122.40
3	D	226	ASP	O-C-N	-5.67	114.80	121.32
3	D	273	ARG	CA-C-O	-5.67	115.05	121.00
1	A	4	DC	P-O5'-C5'	-5.66	111.51	120.00
2	B	24	DC	O3'-P-O5'	-5.60	95.60	104.00
1	A	5	DT	C4-C5-C7	-5.60	114.00	122.40
3	D	279	GLY	CA-C-N	5.58	131.75	121.70
3	D	279	GLY	C-N-CA	5.58	131.75	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	249	ARG	NE-CZ-NH1	5.57	127.07	121.50
3	C	248	GLN	CA-CB-CG	-5.56	102.97	114.10
3	D	262	SER	N-CA-C	5.50	117.36	111.36
2	B	25	DT	P-O3'-C3'	5.48	128.42	120.20
3	D	265	TYR	N-CA-CB	5.48	118.18	110.12
2	B	35	DA	C3'-C2'-C1'	5.47	109.81	101.60
3	D	226	ASP	N-CA-C	5.47	121.90	109.81
2	B	40	DA	P-O5'-C5'	-5.46	111.81	120.00
2	B	39	DG	O3'-P-O5'	-5.43	95.86	104.00
2	B	26	DG	C2'-C3'-O3'	5.42	119.63	111.50
3	C	250	MET	CG-SD-CE	5.39	112.77	100.90
2	B	29	DT	O4'-C1'-C2'	-5.38	98.32	106.40
1	A	9	DA	P-O3'-C3'	5.38	128.26	120.20
2	B	26	DG	C4'-C3'-O3'	-5.33	102.00	110.00
1	A	15	DC	O3'-P-O5'	-5.33	96.00	104.00
3	D	231	LYS	CB-CA-C	-5.32	102.53	110.88
3	D	272	ALA	CA-C-O	5.29	126.03	120.42
3	C	281	ARG	N-CA-C	-5.28	96.21	111.00
3	C	256	LYS	CA-C-O	-5.28	114.93	120.63
1	A	1	DT	O5'-C5'-C4'	5.26	118.69	110.80
3	C	237	GLU	CB-CA-C	-5.24	102.10	110.79
3	C	225	LYS	O-C-N	-5.18	114.72	123.00
2	B	25	DT	C2-N1-C1'	-5.17	111.59	119.35
3	D	245	ARG	N-CA-C	5.16	117.32	111.02
3	C	261	LEU	O-C-N	-5.16	116.27	122.15
3	C	248	GLN	N-CA-C	5.15	116.58	111.07
2	B	37	DA	O5'-C5'-C4'	5.15	118.53	110.80
3	C	273	ARG	CA-C-O	-5.15	115.59	121.00
3	D	234	ARG	NE-CZ-NH2	-5.14	114.57	119.20
3	C	266	HIS	CA-CB-CG	-5.13	108.67	113.80
3	D	225	LYS	CA-C-O	5.12	127.84	120.51
2	B	23	DA	C3'-C2'-C1'	-5.11	93.94	101.60
3	C	280	GLU	CA-CB-CG	5.09	124.29	114.10
3	D	240	ARG	N-CA-C	5.09	117.49	111.33
3	C	280	GLU	N-CA-C	-5.07	101.42	109.59
2	B	26	DG	C4'-C3'-C2'	-5.06	94.81	102.40
3	C	227	PRO	O-C-N	-5.06	116.05	122.17
1	A	2	DT	N1-C1'-C2'	5.04	121.06	113.50
1	A	19	DT	C5'-C4'-C3'	-5.03	107.35	114.90
3	C	244	ALA	CA-C-O	5.03	126.06	120.63

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	40	DA	Sidechain

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	399	0	230	7	0
2	B	415	0	222	12	0
3	C	472	0	506	18	0
3	D	469	0	502	19	0
4	A	4	0	0	0	0
4	B	2	0	0	0	0
4	C	4	0	0	0	0
4	D	7	0	0	0	0
All	All	1772	0	1460	43	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 13.

All (43) 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:C:261:LEU:HG	3:D:260:LEU:HD21	1.50	0.89
3:C:256:LYS:O	3:C:260:LEU:HG	1.83	0.76
3:C:257:VAL:O	3:C:261:LEU:HD12	1.87	0.74
3:D:226:ASP:HB2	3:D:229:ALA:HB3	1.68	0.73
2:B:23:DA:C8	2:B:24:DC:H5	2.12	0.67
3:C:227:PRO:O	3:C:231:LYS:HB2	1.98	0.63
3:D:237:GLU:HB3	3:D:241:ARG:HH12	1.65	0.62
3:D:275:LYS:HE3	3:D:280:GLU:HA	1.81	0.61
3:D:249:ARG:HG3	3:D:249:ARG:HH11	1.68	0.58
3:D:245:ARG:HD2	3:D:249:ARG:HH21	1.68	0.57
2:B:28:DA:P	3:C:241:ARG:HH22	2.28	0.56
1:A:12:DC:H2''	1:A:13:DA:C8	2.41	0.55
1:A:10:DC:H42	2:B:32:DG:H1	1.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:250:MET:O	3:C:250:MET:HG2	2.09	0.52
3:C:271:VAL:HG22	3:D:271:VAL:HG23	1.92	0.52
3:C:277:LEU:HD12	3:D:278:VAL:HG11	1.93	0.51
2:B:23:DA:H8	2:B:24:DC:H5	1.54	0.51
3:C:264:ASN:HB2	3:D:264:ASN:HD21	1.75	0.50
1:A:13:DA:H2''	1:A:14:DT:H5''	1.93	0.50
2:B:32:DG:OP1	3:D:240:ARG:NH2	2.47	0.48
3:D:245:ARG:HD2	3:D:249:ARG:NH2	2.28	0.48
3:C:253:LEU:HD23	3:C:256:LYS:NZ	2.29	0.48
3:C:277:LEU:HD23	3:C:277:LEU:H	1.78	0.46
3:C:267:LEU:HB3	3:D:267:LEU:HD23	1.97	0.46
2:B:23:DA:H2''	2:B:24:DC:OP2	2.14	0.46
1:A:12:DC:OP2	3:C:232:ARG:HD2	2.15	0.46
2:B:25:DT:H2''	2:B:26:DG:H5'	1.99	0.45
2:B:32:DG:N7	3:D:243:ARG:NH2	2.62	0.45
3:C:274:LEU:HD11	3:D:275:LYS:HZ2	1.80	0.45
1:A:5:DT:H2''	1:A:6:DA:C8	2.52	0.45
3:D:237:GLU:HB3	3:D:241:ARG:NH1	2.32	0.44
2:B:21:DA:H1'	2:B:22:DA:OP2	2.18	0.44
3:D:257:VAL:O	3:D:261:LEU:HG	2.18	0.43
3:C:264:ASN:CB	3:D:264:ASN:HD21	2.33	0.42
3:C:278:VAL:HG13	3:C:279:GLY:H	1.84	0.42
3:D:264:ASN:HD22	3:D:264:ASN:N	2.18	0.42
3:D:261:LEU:HD23	3:D:261:LEU:HA	1.89	0.41
3:C:245:ARG:HH11	3:C:245:ARG:HD3	1.69	0.41
2:B:38:DG:H1'	2:B:39:DG:H5'	2.02	0.41
2:B:39:DG:O5'	2:B:39:DG:H2'	2.21	0.41
1:A:9:DA:H2'	3:C:243:ARG:NH1	2.36	0.41
2:B:26:DG:H1'	2:B:27:DG:C8	2.55	0.41
1:A:1:DT:H2''	1:A:2:DT:O5'	2.21	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	
3	C	55/58 (95%)	48 (87%)	6 (11%)	1 (2%)	6	25
3	D	55/58 (95%)	49 (89%)	4 (7%)	2 (4%)	2	11
All	All	110/116 (95%)	97 (88%)	10 (9%)	3 (3%)	4	16

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	278	VAL
3	D	226	ASP
3	D	227	PRO

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	C	49/50 (98%)	41 (84%)	8 (16%)	2	8
3	D	49/50 (98%)	38 (78%)	11 (22%)	1	3
All	All	98/100 (98%)	79 (81%)	19 (19%)	1	5

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	231	LYS
3	C	232	ARG
3	C	248	GLN
3	C	253	LEU
3	C	263	LYS
3	C	264	ASN
3	C	276	LYS
3	C	278	VAL
3	D	225	LYS
3	D	242	SER

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Mol	Chain	Res	Type
3	D	247	LEU
3	D	248	GLN
3	D	249	ARG
3	D	256	LYS
3	D	258	GLU
3	D	262	SER
3	D	267	LEU
3	D	270	GLU
3	D	276	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	269	ASN
3	D	252	GLN
3	D	264	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](#)

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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.