



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:35 PM UTC

PDB ID : 1APL / pdb_00001apl
Title : CRYSTAL STRUCTURE OF A MAT-ALPHA2 HOMEODOMAIN-
OPERATOR COMPLEX SUGGESTS A GENERAL MODEL FOR
HOMEODOMAIN-DNA INTERACTIONS
Authors : Wolberger, C.; Vershon, A.K.; Liu, B.; Johnson, A.D.; Pabo, C.O.
Deposited on : 1993-10-04
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 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

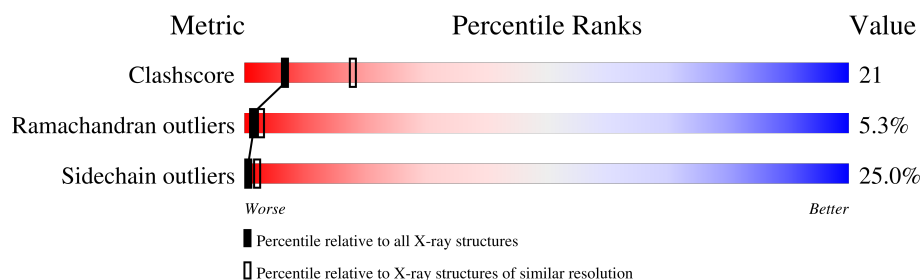
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (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 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	21	5% 48% 43% 5%
2	B	21	43% 38% 19%
3	C	83	24% 37% 5% 5% 29%
3	D	83	24% 24% 12% 10% 30%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1791 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(*AP*CP*AP*TP*GP*TP*AP*AP*TP*TP*CP*AP*TP*TP*TP*AP*C P*AP*CP*GP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	21	Total	C	N	O	P	0	0	0
			423	205	74	124	20			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	21	Total	C	N	O	P	0	0	0
			432	208	80	124	20			

- Molecule 3 is a protein called PROTEIN (MAT-ALPHA2 HOMEODOMAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	59	Total	C	N	O	S	0	0	0
			480	298	93	88	1			
3	D	58	Total	C	N	O	S	0	0	0
			456	286	86	83	1			

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(*AP*CP*AP*TP*GP*TP*AP*AP*TP*TP*CP*AP*TP*TP*TP*AP*C P*AP*CP*GP*C)-3')

Chain A: 



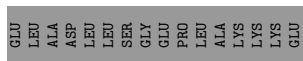
- Molecule 2: DNA (5'-D(*TP*GP*CP*GP*TP*GP*TP*AP*AP*AP*TP*GP*AP*AP*TP*TP*A P*CP*AP*TP*G)-3')

Chain B: 



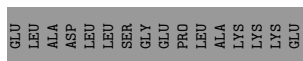
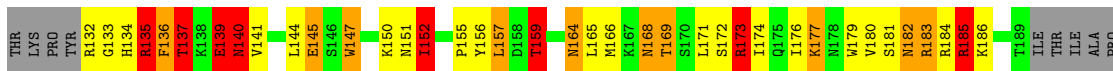
- Molecule 3: PROTEIN (MAT-ALPHA2 HOMEODOMAIN)

Chain C: 



- Molecule 3: PROTEIN (MAT-ALPHA2 HOMEODOMAIN)

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 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	60.78Å 39.93Å 68.79Å 90.00° 97.35° 90.00°	Depositor
Resolution (Å)	8.00 – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.226 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1791	wwPDB-VP
Average B, all atoms (Å ²)	35.0	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	1.22	1/473 (0.2%)	3.49	52/727 (7.2%)
2	B	1.14	0/485	3.89	48/748 (6.4%)
3	C	1.28	3/487 (0.6%)	2.29	23/656 (3.5%)
3	D	1.24	1/463 (0.2%)	2.36	23/626 (3.7%)
All	All	1.22	5/1908 (0.3%)	3.14	146/2757 (5.3%)

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
1	A	0	4
2	B	0	5
3	D	0	1
All	All	0	10

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	155	PRO	CA-CB	-6.83	1.48	1.53
3	C	135	ARG	CZ-NH2	6.08	1.41	1.33
3	D	140	ASN	CA-C	-5.34	1.45	1.52
3	C	135	ARG	CZ-NH1	5.10	1.39	1.32
1	A	6	DT	O3'-P	5.08	1.68	1.61

All (146) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	32	DT	O3'-P-O5'	42.52	167.78	104.00
2	B	29	DA	O3'-P-O5'	33.00	153.51	104.00
2	B	27	DG	O3'-P-O5'	32.77	153.15	104.00
1	A	16	DA	O3'-P-O5'	-31.78	56.33	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	DA	O3'-P-O5'	25.98	142.97	104.00
1	A	5	DG	O3'-P-O5'	-25.46	65.81	104.00
2	B	25	DG	O3'-P-O5'	-24.53	67.20	104.00
2	B	36	DT	O3'-P-O5'	22.01	137.01	104.00
1	A	6	DT	O3'-P-O5'	21.15	135.73	104.00
1	A	3	DA	O3'-P-O5'	-19.42	74.87	104.00
1	A	17	DC	O3'-P-O5'	18.98	132.47	104.00
2	B	38	DA	O3'-P-O5'	-18.48	76.28	104.00
1	A	7	DA	O3'-P-O5'	-17.41	77.89	104.00
2	B	28	DT	OP1-P-O3'	-17.12	56.63	108.00
1	A	13	DT	O3'-P-O5'	-16.48	79.28	104.00
1	A	10	DT	O3'-P-O5'	15.60	127.39	104.00
2	B	29	DA	OP1-P-O3'	-15.40	61.78	108.00
2	B	32	DT	OP1-P-O3'	-14.12	65.63	108.00
1	A	10	DT	OP2-P-O3'	-13.85	66.44	108.00
2	B	41	DT	OP1-P-O3'	-13.73	66.81	108.00
2	B	34	DA	O3'-P-O5'	-13.45	83.83	104.00
2	B	39	DC	O3'-P-O5'	13.35	124.02	104.00
2	B	41	DT	OP2-P-O3'	12.94	146.82	108.00
2	B	37	DT	O3'-P-O5'	-12.84	84.75	104.00
1	A	20	DG	O3'-P-O5'	-12.59	85.11	104.00
1	A	11	DC	OP2-P-O3'	12.30	144.92	108.00
2	B	25	DG	OP1-P-O3'	12.13	144.40	108.00
2	B	22	DT	O3'-P-O5'	11.75	121.62	104.00
3	C	164	ASN	CA-CB-CG	-11.55	101.05	112.60
2	B	35	DA	O3'-P-O5'	-11.00	87.50	104.00
1	A	6	DT	OP2-P-O3'	-10.84	75.48	108.00
2	B	39	DC	OP1-P-O3'	-10.49	76.53	108.00
3	C	151	ASN	OD1-CG-ND2	-10.39	112.21	122.60
2	B	28	DT	O3'-P-O5'	-10.03	88.95	104.00
2	B	40	DA	P-O5'-C5'	8.97	133.46	120.00
1	A	19	DC	OP2-P-O3'	8.96	134.89	108.00
1	A	11	DC	OP1-P-O3'	-8.95	81.16	108.00
1	A	16	DA	OP1-P-O3'	-8.89	81.32	108.00
3	D	136	PHE	CA-CB-CG	8.83	122.63	113.80
3	D	140	ASN	CA-CB-CG	-8.65	103.95	112.60
2	B	27	DG	OP1-P-O3'	-8.54	82.37	108.00
1	A	9	DT	OP2-P-O3'	8.51	133.52	108.00
1	A	11	DC	O3'-P-O5'	-8.41	91.39	104.00
1	A	19	DC	OP1-P-O3'	-8.36	82.92	108.00
2	B	26	DT	OP1-P-O3'	-8.03	83.91	108.00
1	A	3	DA	OP1-P-O3'	7.82	131.47	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	6	DT	O4'-C1'-C2'	-7.77	94.74	106.40
1	A	17	DC	OP1-P-O3'	-7.66	85.01	108.00
2	B	37	DT	C1'-O4'-C4'	-7.61	98.28	109.70
1	A	20	DG	OP2-P-O3'	7.59	130.76	108.00
2	B	32	DT	OP2-P-O3'	-7.56	85.31	108.00
1	A	1	DA	OP2-P-O3'	-7.54	85.39	108.00
3	D	139	GLU	N-CA-C	-7.29	95.69	108.23
2	B	33	DG	OP2-P-O3'	-7.22	86.35	108.00
1	A	8	DA	C4'-C3'-O3'	-7.19	99.21	110.00
1	A	9	DT	OP1-P-O3'	-7.18	86.46	108.00
1	A	15	DT	OP2-P-O3'	-7.10	86.71	108.00
3	C	181	SER	CA-CB-OG	7.06	125.22	111.10
2	B	27	DG	OP2-P-O3'	-7.05	86.86	108.00
2	B	22	DT	OP1-P-O3'	-7.04	86.88	108.00
2	B	26	DT	OP2-P-O3'	6.97	128.92	108.00
3	D	132	ARG	N-CA-C	-6.97	91.48	111.00
1	A	19	DC	O3'-P-O5'	-6.95	93.58	104.00
3	C	135	ARG	N-CA-C	6.94	120.55	110.28
3	D	159	THR	N-CA-C	6.88	125.45	110.80
1	A	11	DC	P-O5'-C5'	-6.82	109.78	120.00
3	C	183	ARG	NE-CZ-NH2	-6.78	113.10	119.20
2	B	34	DA	OP2-P-O3'	6.75	128.26	108.00
1	A	17	DC	P-O5'-C5'	-6.67	109.99	120.00
2	B	22	DT	P-O3'-C3'	-6.67	110.19	120.20
1	A	7	DA	OP2-P-O3'	6.63	127.89	108.00
3	D	137	THR	N-CA-C	6.63	119.63	110.35
3	C	184	ARG	CA-CB-CG	-6.62	100.86	114.10
2	B	24	DC	O3'-P-O5'	6.61	113.92	104.00
1	A	11	DC	C5'-C4'-C3'	-6.60	105.00	114.90
2	B	34	DA	O4'-C1'-C2'	-6.57	96.55	106.40
1	A	1	DA	OP1-P-O3'	-6.57	88.30	108.00
3	D	135	ARG	CA-CB-CG	-6.54	101.02	114.10
3	D	150	LYS	N-CA-C	-6.49	102.87	111.24
3	D	182	ASN	CA-CB-CG	6.43	119.03	112.60
3	D	179	TRP	N-CA-C	-6.36	104.35	111.28
1	A	12	DA	OP1-P-O3'	-6.35	88.96	108.00
2	B	28	DT	P-O5'-C5'	6.27	129.40	120.00
2	B	23	DG	OP1-P-O3'	-6.25	89.26	108.00
2	B	33	DG	O3'-P-O5'	6.19	113.29	104.00
2	B	33	DG	O5'-C5'-C4'	6.17	120.05	110.80
1	A	6	DT	C1'-O4'-C4'	-6.16	100.46	109.70
3	D	135	ARG	N-CA-C	6.12	118.61	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	25	DG	P-O5'-C5'	-6.02	110.97	120.00
2	B	30	DA	C1'-O4'-C4'	-6.02	100.68	109.70
1	A	10	DT	O4'-C4'-C3'	-5.99	96.41	105.40
2	B	38	DA	C4'-C3'-O3'	-5.93	101.10	110.00
1	A	5	DG	O4'-C1'-C2'	-5.92	97.52	106.40
3	C	182	ASN	CA-CB-CG	5.90	118.50	112.60
3	C	137	THR	CA-CB-OG1	-5.87	100.79	109.60
3	C	137	THR	N-CA-CB	-5.84	100.40	109.34
1	A	15	DT	P-O3'-C3'	5.84	128.95	120.20
2	B	37	DT	OP1-P-O3'	5.82	125.45	108.00
1	A	16	DA	O4'-C1'-C2'	-5.72	97.82	106.40
1	A	2	DC	C4'-C3'-O3'	-5.71	101.44	110.00
1	A	12	DA	O4'-C1'-C2'	-5.71	97.84	106.40
1	A	2	DC	C4'-C3'-C2'	-5.71	93.84	102.40
3	C	156	TYR	N-CA-C	-5.70	100.11	109.40
3	D	181	SER	N-CA-C	5.66	117.13	111.07
3	D	134	HIS	CB-CA-C	-5.62	101.75	111.30
3	C	134	HIS	CB-CA-C	-5.60	99.28	110.42
3	C	152	ILE	CB-CA-C	-5.51	99.26	111.77
1	A	13	DT	C4'-C3'-O3'	-5.51	101.73	110.00
3	D	179	TRP	CB-CG-CD1	-5.50	118.65	126.90
1	A	15	DT	OP1-P-O3'	5.49	124.47	108.00
3	C	151	ASN	CB-CG-ND2	5.48	124.62	116.40
3	D	139	GLU	N-CA-CB	5.47	118.17	110.24
3	D	168	ASN	CA-CB-CG	-5.46	107.14	112.60
3	C	137	THR	CB-CA-C	5.46	117.30	109.71
3	D	182	ASN	N-CA-C	-5.45	105.33	111.28
2	B	33	DG	OP1-P-O3'	5.45	124.35	108.00
3	C	153	GLU	N-CA-C	5.44	118.13	111.82
3	D	182	ASN	OD1-CG-ND2	-5.44	117.16	122.60
1	A	14	DT	C4-C5-C7	-5.42	114.27	122.40
3	C	135	ARG	N-CA-CB	-5.39	102.05	109.97
3	C	147	TRP	CA-C-O	-5.38	115.16	120.70
3	C	141	VAL	CG1-CB-CG2	-5.38	98.97	110.80
2	B	27	DG	O4'-C1'-C2'	-5.36	98.37	106.40
3	D	151	ASN	N-CA-C	5.36	120.76	113.37
2	B	23	DG	C1'-O4'-C4'	-5.33	101.71	109.70
2	B	28	DT	C1'-O4'-C4'	-5.31	101.73	109.70
3	C	134	HIS	N-CA-CB	5.29	119.43	110.49
3	D	134	HIS	N-CA-CB	5.29	118.23	110.35
3	C	182	ASN	OD1-CG-ND2	-5.24	117.36	122.60
1	A	3	DA	P-O5'-C5'	-5.24	112.14	120.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	24	DC	C4'-C3'-O3'	-5.24	102.14	110.00
3	C	140	ASN	CB-CG-ND2	5.24	124.25	116.40
2	B	33	DG	C1'-O4'-C4'	-5.21	101.88	109.70
3	D	147	TRP	CG-CD2-CE3	5.18	139.08	133.90
3	C	137	THR	CA-CB-CG2	5.17	119.29	110.50
2	B	39	DC	O5'-C5'-C4'	-5.16	103.07	110.80
3	C	131	TYR	N-CA-C	-5.13	96.62	111.00
3	D	179	TRP	CG-CD2-CE3	5.12	139.03	133.90
1	A	5	DG	OP2-P-O3'	5.11	123.32	108.00
3	D	173	ARG	N-CA-C	5.09	121.64	110.80
2	B	25	DG	OP2-P-O3'	-5.09	92.74	108.00
1	A	6	DT	P-O3'-C3'	5.08	127.82	120.20
1	A	6	DT	O4'-C1'-N1	5.08	116.02	108.40
1	A	8	DA	O3'-P-O5'	-5.08	96.39	104.00
1	A	2	DC	O4'-C1'-C2'	-5.03	98.86	106.40
1	A	2	DC	OP1-P-O3'	5.03	123.08	108.00

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	DA	Sidechain
1	A	10	DT	Sidechain
1	A	19	DC	Sidechain
1	A	4	DT	Sidechain
2	B	26	DT	Sidechain
2	B	28	DT	Sidechain
2	B	36	DT	Sidechain
2	B	39	DC	Sidechain
2	B	40	DA	Sidechain
3	D	185	ARG	Sidechain

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	A	423	0	238	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	432	0	240	17	0
3	C	480	0	464	27	0
3	D	456	0	434	28	0
All	All	1791	0	1376	67	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 21.

All (67) 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:B:23:DG:P	3:C:177:LYS:HZ3	1.85	0.99
3:C:173:ARG:NH2	3:C:177:LYS:HZ2	1.62	0.98
2:B:23:DG:P	3:C:177:LYS:NZ	2.36	0.97
3:D:173:ARG:HH12	3:D:177:LYS:HD2	1.39	0.88
2:B:23:DG:OP2	3:C:177:LYS:NZ	2.11	0.84
3:C:173:ARG:NH2	3:C:177:LYS:NZ	2.31	0.78
3:C:173:ARG:HH22	3:C:177:LYS:HZ2	1.36	0.69
3:C:157:LEU:HD21	3:C:180:VAL:HG21	1.77	0.67
3:C:166:MET:SD	3:C:173:ARG:HG3	2.35	0.66
2:B:37:DT:H5'	3:D:135:ARG:HA	1.78	0.65
3:D:165:LEU:O	3:D:169:THR:HB	1.97	0.64
3:C:152:ILE:H	3:C:152:ILE:HD12	1.62	0.64
2:B:29:DA:P	2:B:29:DA:H3'	2.41	0.61
1:A:15:DT:H2''	1:A:16:DA:O5'	2.00	0.61
2:B:29:DA:H3'	2:B:29:DA:OP2	2.02	0.60
1:A:2:DC:H5''	3:D:156:TYR:HE2	1.66	0.59
3:D:169:THR:HG23	3:D:171:LEU:HG	1.86	0.58
3:C:169:THR:HB	3:C:171:LEU:HD23	1.87	0.57
3:C:139:GLU:HG3	3:C:142:ARG:NH1	2.21	0.56
2:B:25:DG:H2''	2:B:26:DT:C6	2.41	0.56
2:B:39:DC:H2'	2:B:40:DA:C8	2.40	0.56
3:C:155:PRO:HG2	3:C:184:ARG:HD3	1.86	0.55
1:A:10:DT:H1'	3:D:135:ARG:NH1	2.22	0.55
2:B:23:DG:P	3:C:177:LYS:HZ1	2.29	0.54
3:D:141:VAL:O	3:D:145:GLU:HB2	2.07	0.54
2:B:25:DG:OP2	3:C:184:ARG:NH1	2.40	0.54
3:C:148:PHE:CD2	3:C:183:ARG:HG3	2.43	0.53
3:D:157:LEU:HD11	3:D:176:ILE:HG22	1.90	0.53
2:B:28:DT:H2'	2:B:29:DA:C8	2.43	0.52
1:A:4:DT:H2'	1:A:5:DG:C8	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:176:ILE:O	3:D:180:VAL:HG23	2.11	0.51
3:D:137:THR:O	3:D:140:ASN:HB2	2.11	0.51
1:A:16:DA:H1'	3:C:131:TYR:N	2.26	0.50
3:D:168:ASN:ND2	3:D:168:ASN:H	2.08	0.50
3:D:133:GLY:O	3:D:135:ARG:HD2	2.11	0.50
3:D:186:LYS:HG2	3:D:186:LYS:O	2.12	0.50
1:A:15:DT:H5''	3:C:136:PHE:CE1	2.46	0.49
3:C:148:PHE:CE2	3:C:183:ARG:HG3	2.47	0.49
3:C:144:LEU:HD23	3:C:165:LEU:HD22	1.95	0.48
1:A:18:DA:H61	2:B:26:DT:H3	1.61	0.48
2:B:35:DA:H2	3:D:135:ARG:HH12	1.62	0.47
1:A:2:DC:OP1	3:D:156:TYR:HD2	1.98	0.47
2:B:30:DA:H2''	2:B:31:DA:O5'	2.15	0.46
2:B:23:DG:OP1	3:C:177:LYS:NZ	2.44	0.45
1:A:17:DC:H2'	1:A:18:DA:C8	2.51	0.45
3:D:169:THR:HG22	3:D:171:LEU:H	1.82	0.45
3:C:165:LEU:HB3	3:C:176:ILE:HD13	1.99	0.45
3:D:174:ILE:O	3:D:177:LYS:HB3	2.17	0.44
1:A:3:DA:OP2	3:D:184:ARG:NH1	2.48	0.44
3:D:152:ILE:O	3:D:155:PRO:HD3	2.18	0.44
3:D:164:ASN:HD22	3:D:164:ASN:HA	1.73	0.44
3:C:153:GLU:HG2	3:C:154:ASN:N	2.33	0.43
3:C:169:THR:HB	3:C:171:LEU:CD2	2.49	0.43
3:C:179:TRP:CZ3	3:C:183:ARG:HG2	2.53	0.43
2:B:25:DG:H2''	2:B:26:DT:H6	1.83	0.42
2:B:41:DT:H2'	2:B:42:DG:C8	2.54	0.42
1:A:16:DA:N3	3:C:131:TYR:HA	2.34	0.42
3:D:137:THR:HB	3:D:139:GLU:O	2.20	0.42
3:D:145:GLU:OE2	3:D:183:ARG:HD3	2.19	0.42
3:C:139:GLU:O	3:C:143:ILE:HG13	2.20	0.41
3:D:144:LEU:HD21	3:D:176:ILE:HG23	2.02	0.41
3:D:182:ASN:OD1	3:D:185:ARG:NH2	2.52	0.41
3:D:173:ARG:NH1	3:D:177:LYS:HD2	2.20	0.41
3:D:147:TRP:CZ2	3:D:157:LEU:HD23	2.56	0.41
3:C:152:ILE:HD12	3:C:152:ILE:N	2.30	0.40
1:A:2:DC:H5''	3:D:156:TYR:CE2	2.52	0.40
3:D:176:ILE:HD12	3:D:176:ILE:H	1.86	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	57/83 (69%)	49 (86%)	7 (12%)	1 (2%)	6	18
3	D	56/83 (68%)	44 (79%)	7 (12%)	5 (9%)	0	0
All	All	113/166 (68%)	93 (82%)	14 (12%)	6 (5%)	1	3

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	173	ARG
3	D	140	ASN
3	D	159	THR
3	D	173	ARG
3	D	157	LEU
3	D	152	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	
3	C	50/76 (66%)	40 (80%)	10 (20%)	1	4
3	D	46/76 (60%)	32 (70%)	14 (30%)	0	1
All	All	96/152 (63%)	72 (75%)	24 (25%)	0	2

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	152	ILE
3	C	155	PRO
3	C	159	THR
3	C	162	LEU
3	C	164	ASN
3	C	173	ARG
3	C	183	ARG
3	C	185	ARG
3	C	188	LYS
3	C	189	THR
3	D	135	ARG
3	D	136	PHE
3	D	137	THR
3	D	139	GLU
3	D	145	GLU
3	D	152	ILE
3	D	159	THR
3	D	164	ASN
3	D	166	MET
3	D	169	THR
3	D	172	SER
3	D	177	LYS
3	D	183	ARG
3	D	185	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	140	ASN
3	C	151	ASN
3	C	164	ASN
3	C	178	ASN
3	D	164	ASN
3	D	168	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

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.