



Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 07:32 pm BST

PDB ID : 1GLU
Title : CRYSTALLOGRAPHIC ANALYSIS OF THE INTERACTION OF THE
GLUCOCORTICOID RECEPTOR WITH DNA
Authors : Luisi, B.F.; Xu, W.X.; Otwinowski, Z.; Freedman, L.P.; Yamamoto, K.R.;
Sigler, P.B.
Deposited on : 1992-08-30
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

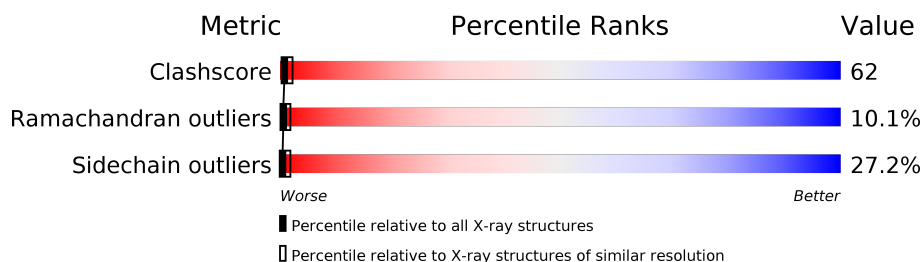
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	19	<div> <div>21%</div> <div>74%</div> <div>5%</div> </div>
1	D	19	<div> <div>16%</div> <div>74%</div> <div>11%</div> </div>
2	A	81	<div> <div>17%</div> <div>33%</div> <div>33%</div> <div>16%</div> </div>
2	B	81	<div> <div>25%</div> <div>42%</div> <div>25%</div> <div>9%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2071 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*AP*GP*AP*AP*CP*AP*TP*CP*GP*AP*TP*GP*TP*TP*C P*TP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	19	Total	C	N	O	P	0	0	0
			385	185	70	112	18			
1	D	19	Total	C	N	O	P	0	0	0
			385	185	70	112	18			

- Molecule 2 is a protein called PROTEIN (GLUCOCORTICOID RECEPTOR).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	81	Total	C	N	O	S	0	0	0
			628	385	124	107	12			
2	B	81	Total	C	N	O	S	0	0	0
			628	385	124	107	12			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	437	ALA	PRO	CONFLICT	UNP P06536
A	438	ARG	LYS	CONFLICT	UNP P06536
A	439	PRO	LEU	CONFLICT	UNP P06536
B	437	ALA	PRO	CONFLICT	UNP P06536
B	438	ARG	LYS	CONFLICT	UNP P06536
B	439	PRO	LEU	CONFLICT	UNP P06536

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Zn	0	0
			2	2		
3	A	2	Total	Zn	0	0
			2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	7	Total 7	O 7	0	0
4	D	9	Total 9	O 9	0	0
4	A	7	Total 7	O 7	0	0
4	B	18	Total 18	O 18	0	0

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

Chain C: 



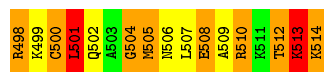
- Molecule 1: DNA (5'-D(*CP*CP*AP*GP*AP*AP*CP*AP*TP*CP*GP*AP*TP*GP*TP*TP*C P*TP*G)-3')

Chain D: 



- Molecule 2: PROTEIN (GLUCOCORTICOID RECEPTOR)

Chain A: 



- Molecule 2: PROTEIN (GLUCOCORTICOID RECEPTOR)

Chain B: 



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	38.50Å 95.70Å 120.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR, PROLSQ	Depositor
R, R_{free}	0.196 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2071	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	C	2.49	23/431 (5.3%)	4.15	124/663 (18.7%)
1	D	2.62	27/431 (6.3%)	4.34	134/663 (20.2%)
2	A	1.01	0/637	2.11	32/848 (3.8%)
2	B	0.99	0/637	2.11	33/848 (3.9%)
All	All	1.80	50/2136 (2.3%)	3.23	323/3022 (10.7%)

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	2
1	D	0	2
2	A	0	10
2	B	0	6
All	All	0	20

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	-9	DC	P-O5'	-14.53	1.45	1.59
1	D	-7	DG	O3'-P	8.93	1.71	1.61
1	C	-7	DG	C4'-O4'	-8.78	1.36	1.45
1	D	-5	DA	O3'-P	8.03	1.70	1.61
1	C	6	DT	P-O5'	7.92	1.67	1.59
1	C	8	DT	P-O5'	7.78	1.67	1.59
1	D	-5	DA	P-O5'	7.69	1.67	1.59
1	D	-6	DA	P-O5'	7.51	1.67	1.59
1	D	2	DA	P-O5'	7.44	1.67	1.59
1	D	7	DC	O3'-P	7.34	1.70	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	-7	DG	C5'-C4'	-7.05	1.43	1.51
1	D	-9	DC	O3'-P	7.03	1.69	1.61
1	C	2	DA	P-O5'	6.94	1.66	1.59
1	C	1	DG	C8-N7	6.85	1.35	1.30
1	D	9	DG	P-O5'	6.84	1.66	1.59
1	C	-9	DC	C4'-O4'	-6.82	1.38	1.45
1	C	-6	DA	C4'-O4'	-6.78	1.38	1.45
1	D	8	DT	C4'-O4'	-6.60	1.38	1.45
1	C	1	DG	P-O5'	6.45	1.66	1.59
1	D	1	DG	P-OP1	6.41	1.59	1.49
1	C	-10	DC	C4'-O4'	-6.40	1.38	1.45
1	D	3	DT	O3'-P	6.39	1.68	1.61
1	D	-10	DC	O3'-P	6.33	1.68	1.61
1	C	3	DT	C4-O4	6.31	1.28	1.23
1	D	7	DC	P-O5'	6.29	1.66	1.59
1	C	6	DT	O3'-P	6.27	1.68	1.61
1	C	1	DG	O3'-P	6.05	1.68	1.61
1	D	4	DG	C4'-O4'	-6.01	1.39	1.45
1	C	-9	DC	C5'-C4'	-5.96	1.44	1.51
1	D	2	DA	O3'-P	5.89	1.68	1.61
1	C	-1	DC	C4'-O4'	-5.80	1.39	1.45
1	C	3	DT	O3'-P	5.79	1.68	1.61
1	D	-6	DA	C8-N7	5.68	1.35	1.31
1	D	7	DC	P-OP2	5.68	1.58	1.49
1	D	-9	DC	P-OP2	5.67	1.58	1.49
1	D	8	DT	P-O5'	5.67	1.65	1.59
1	D	8	DT	C4-O4	5.57	1.28	1.23
1	D	-2	DT	O3'-P	5.49	1.67	1.61
1	C	-8	DA	P-OP1	5.49	1.58	1.49
1	C	-9	DC	P-O5'	5.42	1.65	1.59
1	D	-8	DA	P-O5'	5.42	1.65	1.59
1	D	-2	DT	P-O5'	5.30	1.65	1.59
1	D	1	DG	O3'-P	5.30	1.67	1.61
1	C	-3	DA	N1-C2	5.19	1.39	1.34
1	C	-5	DA	O3'-P	5.19	1.67	1.61
1	C	8	DT	C4-C5	-5.16	1.40	1.45
1	C	8	DT	C4'-O4'	-5.14	1.40	1.45
1	D	9	DG	C4'-O4'	-5.05	1.40	1.45
1	C	9	DG	C4'-O4'	-5.05	1.40	1.45
1	D	7	DC	C5'-C4'	-5.01	1.45	1.51

All (323) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	-10	DC	P-O3'-C3'	21.88	145.96	119.70
1	D	-5	DA	O4'-C1'-N9	19.24	121.47	108.00
1	C	-3	DA	O4'-C1'-N9	17.65	120.36	108.00
1	C	4	DG	O5'-P-OP2	17.35	131.52	110.70
1	D	-10	DC	O4'-C1'-N1	17.34	120.14	108.00
1	D	-9	DC	O5'-P-OP1	16.79	130.84	110.70
1	C	8	DT	O4'-C1'-N1	16.26	119.39	108.00
1	C	-6	DA	P-O5'-C5'	-15.19	96.60	120.90
1	D	-5	DA	P-O3'-C3'	-14.43	102.39	119.70
2	B	496	ARG	NE-CZ-NH2	14.37	127.48	120.30
1	D	6	DT	P-O3'-C3'	14.34	136.91	119.70
1	C	5	DT	C2-N3-C4	-13.83	118.90	127.20
2	A	479	ARG	NE-CZ-NH1	13.30	126.95	120.30
1	C	-1	DC	P-O5'-C5'	-13.26	99.68	120.90
1	D	2	DA	O5'-P-OP2	12.64	125.87	110.70
1	D	8	DT	O4'-C1'-N1	-12.60	99.18	108.00
1	D	8	DT	P-O5'-C5'	-12.57	100.80	120.90
1	C	-5	DA	P-O3'-C3'	-12.52	104.67	119.70
1	D	3	DT	O5'-P-OP2	12.43	125.62	110.70
1	C	1	DG	P-O5'-C5'	-12.43	101.01	120.90
1	C	6	DT	O5'-P-OP2	12.35	125.52	110.70
1	D	3	DT	C2-N3-C4	-12.19	119.89	127.20
1	D	-10	DC	P-O3'-C3'	-12.12	105.16	119.70
1	D	-5	DA	P-O5'-C5'	-11.89	101.87	120.90
1	C	5	DT	P-O3'-C3'	11.89	133.97	119.70
2	A	496	ARG	NE-CZ-NH1	11.86	126.23	120.30
2	B	450	CYS	O-C-N	-11.49	104.32	122.70
1	D	-6	DA	P-O5'-C5'	-11.43	102.61	120.90
1	D	-7	DG	P-O5'-C5'	-11.37	102.70	120.90
1	D	2	DA	P-O5'-C5'	-11.37	102.72	120.90
1	C	-7	DG	P-O5'-C5'	-11.35	102.74	120.90
1	D	-9	DC	OP1-P-OP2	-11.30	102.65	119.60
1	C	9	DG	O5'-P-OP2	11.26	124.21	110.70
1	D	4	DG	N1-C6-O6	-11.18	113.19	119.90
1	D	9	DG	O4'-C1'-N9	11.16	115.81	108.00
2	B	496	ARG	NE-CZ-NH1	-11.09	114.75	120.30
2	B	489	ARG	NE-CZ-NH2	-11.01	114.80	120.30
1	C	9	DG	OP1-P-OP2	-11.00	103.10	119.60
1	D	2	DA	P-O3'-C3'	-10.80	106.74	119.70
1	C	3	DT	P-O3'-C3'	-10.75	106.80	119.70
1	D	5	DT	P-O5'-C5'	-10.71	103.76	120.90
1	D	7	DC	P-O5'-C5'	-10.52	104.07	120.90
1	D	6	DT	C2-N3-C4	-10.48	120.91	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1	DG	P-O5'-C5'	-10.42	104.23	120.90
1	C	2	DA	O3'-P-O5'	-10.31	84.40	104.00
1	D	7	DC	O4'-C1'-N1	10.30	115.21	108.00
1	D	4	DG	P-O3'-C3'	-10.23	107.42	119.70
1	D	8	DT	C2-N3-C4	-10.09	121.15	127.20
1	D	5	DT	C2-N3-C4	-9.97	121.22	127.20
1	D	-1	DC	OP2-P-O3'	9.92	127.02	105.20
1	C	9	DG	O4'-C1'-N9	9.90	114.93	108.00
1	C	-6	DA	N1-C2-N3	-9.83	124.39	129.30
1	C	-1	DC	P-O3'-C3'	-9.82	107.92	119.70
1	D	8	DT	P-O3'-C3'	-9.82	107.92	119.70
1	D	7	DC	P-O3'-C3'	-9.78	107.97	119.70
1	C	-6	DA	C5'-C4'-O4'	9.74	127.81	109.30
1	D	3	DT	P-O3'-C3'	-9.64	108.13	119.70
1	D	-8	DA	P-O3'-C3'	-9.63	108.15	119.70
1	C	6	DT	C2-N3-C4	-9.61	121.43	127.20
1	D	7	DC	O5'-P-OP1	9.60	122.22	110.70
1	C	8	DT	C2-N3-C4	-9.57	121.46	127.20
1	D	6	DT	N3-C4-O4	-9.36	114.29	119.90
1	C	3	DT	O5'-P-OP2	9.29	121.84	110.70
1	C	9	DG	C6-N1-C2	-9.26	119.54	125.10
1	D	5	DT	O4'-C1'-N1	9.19	114.43	108.00
1	D	3	DT	N3-C4-C5	9.17	120.70	115.20
1	C	-9	DC	P-O5'-C5'	-9.12	106.31	120.90
1	C	-4	DC	O4'-C4'-C3'	9.06	111.44	106.00
1	C	6	DT	P-O3'-C3'	9.02	130.53	119.70
1	D	-1	DC	O5'-P-OP2	9.02	121.53	110.70
1	D	6	DT	O4'-C1'-N1	9.02	114.31	108.00
1	D	-8	DA	P-O5'-C5'	-9.00	106.50	120.90
2	B	446	GLU	CA-CB-CG	8.92	133.03	113.40
1	C	8	DT	N3-C4-C5	8.92	120.55	115.20
1	C	5	DT	N3-C4-C5	8.75	120.45	115.20
1	C	-2	DT	P-O3'-C3'	8.71	130.16	119.70
1	D	-7	DG	C6-N1-C2	-8.66	119.91	125.10
1	D	8	DT	C5'-C4'-C3'	8.56	129.50	114.10
1	C	-3	DA	OP1-P-OP2	-8.51	106.84	119.60
1	D	-1	DC	OP1-P-O3'	-8.47	86.58	105.20
1	C	1	DG	C6-N1-C2	-8.41	120.06	125.10
1	D	4	DG	P-O5'-C5'	-8.39	107.47	120.90
1	D	-4	DC	O5'-P-OP1	8.36	120.73	110.70
1	D	-10	DC	O4'-C1'-C2'	-8.34	99.23	105.90
1	D	9	DG	P-O5'-C5'	-8.32	107.58	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	3	DT	O4'-C1'-N1	8.31	113.82	108.00
1	C	-8	DA	O4'-C1'-N9	8.29	113.80	108.00
1	D	3	DT	N3-C4-O4	-8.29	114.93	119.90
1	D	-8	DA	OP1-P-OP2	8.26	131.98	119.60
1	D	-1	DC	N3-C4-C5	-8.20	118.62	121.90
1	D	8	DT	N3-C4-C5	8.18	120.11	115.20
1	C	3	DT	O4'-C1'-N1	8.16	113.72	108.00
1	D	-2	DT	C2-N3-C4	-8.15	122.31	127.20
1	D	-7	DG	P-O3'-C3'	-8.13	109.95	119.70
2	A	435	LYS	CB-CA-C	8.05	126.49	110.40
1	C	-2	DT	O4'-C1'-C2'	-8.02	99.49	105.90
1	C	-3	DA	C5-C6-N1	-7.93	113.73	117.70
1	C	-8	DA	P-O5'-C5'	-7.92	108.22	120.90
1	C	-2	DT	C2-N3-C4	-7.89	122.47	127.20
2	A	438	ARG	NE-CZ-NH2	7.87	124.23	120.30
1	C	-7	DG	C5'-C4'-C3'	7.86	128.25	114.10
1	D	5	DT	N1-C2-N3	7.85	119.31	114.60
2	B	510	ARG	NE-CZ-NH2	-7.84	116.38	120.30
1	D	3	DT	P-O5'-C5'	-7.83	108.37	120.90
1	C	-5	DA	N1-C2-N3	-7.82	125.39	129.30
2	B	434	MET	CB-CA-C	7.71	125.82	110.40
1	C	-5	DA	P-O5'-C5'	-7.71	108.57	120.90
1	C	1	DG	O5'-P-OP1	7.70	119.94	110.70
1	D	-3	DA	C5-C6-N1	-7.65	113.87	117.70
1	C	5	DT	N1-C2-N3	7.64	119.18	114.60
1	D	-7	DG	O3'-P-O5'	-7.63	89.50	104.00
1	C	6	DT	P-O5'-C5'	-7.63	108.69	120.90
1	D	6	DT	N1-C2-N3	7.62	119.17	114.60
1	C	6	DT	N1-C2-N3	7.62	119.17	114.60
1	C	-6	DA	P-O3'-C3'	-7.61	110.57	119.70
2	B	443	CYS	CB-CA-C	7.60	125.59	110.40
1	D	-4	DC	O4'-C1'-N1	-7.58	102.69	108.00
1	D	3	DT	N1-C2-N3	7.54	119.13	114.60
2	A	510	ARG	NE-CZ-NH2	7.54	124.07	120.30
1	C	4	DG	P-O5'-C5'	-7.54	108.83	120.90
2	A	487	ILE	CG1-CB-CG2	-7.54	94.81	111.40
1	C	4	DG	C6-N1-C2	-7.52	120.59	125.10
1	D	-7	DG	O4'-C1'-N9	7.50	113.25	108.00
1	C	3	DT	O3'-P-O5'	-7.49	89.77	104.00
1	C	-9	DC	O4'-C1'-N1	7.49	113.24	108.00
1	D	9	DG	C5-C6-N1	7.48	115.24	111.50
2	B	438	ARG	NE-CZ-NH2	7.48	124.04	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	434	MET	CG-SD-CE	7.48	112.17	100.20
1	D	-8	DA	N1-C2-N3	-7.48	125.56	129.30
2	A	496	ARG	NE-CZ-NH2	-7.47	116.56	120.30
2	A	479	ARG	C-N-CA	7.46	140.34	121.70
1	C	-4	DC	N1-C1'-C2'	-7.46	98.44	112.60
1	D	-7	DG	C8-N9-C4	-7.44	103.42	106.40
1	D	-9	DC	O5'-C5'-C4'	-7.41	92.48	111.00
1	D	8	DT	N3-C4-O4	-7.41	115.45	119.90
1	C	1	DG	O4'-C1'-C2'	-7.37	100.01	105.90
1	C	8	DT	P-O5'-C5'	-7.37	109.12	120.90
1	C	3	DT	C5'-C4'-O4'	7.36	123.29	109.30
1	D	4	DG	O5'-P-OP2	7.29	119.45	110.70
1	C	5	DT	N3-C4-O4	-7.29	115.53	119.90
1	C	-10	DC	O4'-C1'-C2'	-7.28	100.08	105.90
1	D	-10	DC	N1-C2-O2	7.28	123.27	118.90
1	C	-8	DA	C5-C6-N1	-7.26	114.07	117.70
1	D	-7	DG	C5-C6-N1	7.23	115.12	111.50
1	D	-1	DC	C5-C4-N4	7.22	125.25	120.20
1	C	9	DG	C5-C6-N1	7.22	115.11	111.50
1	C	-10	DC	O4'-C1'-N1	7.21	113.05	108.00
1	C	-5	DA	O4'-C4'-C3'	7.16	110.29	106.00
1	D	8	DT	N1-C2-O2	-7.10	117.42	123.10
1	D	-7	DG	N7-C8-N9	7.09	116.65	113.10
1	C	-2	DT	OP1-P-OP2	-7.08	108.97	119.60
1	D	-2	DT	N3-C2-O2	-7.04	118.07	122.30
2	A	475	LEU	CB-CA-C	-7.04	96.83	110.20
1	D	-2	DT	N3-C4-O4	-7.02	115.69	119.90
1	C	-1	DC	O5'-P-OP1	-7.01	99.39	105.70
1	D	-1	DC	N3-C2-O2	-7.00	117.00	121.90
1	D	5	DT	N3-C4-C5	6.90	119.34	115.20
1	C	-2	DT	N1-C2-N3	6.88	118.73	114.60
2	A	466	ARG	NH1-CZ-NH2	-6.88	111.83	119.40
2	A	469	GLU	CA-CB-CG	6.87	128.51	113.40
2	A	496	ARG	CD-NE-CZ	6.86	133.20	123.60
1	D	6	DT	N3-C2-O2	-6.84	118.19	122.30
1	C	-1	DC	C2'-C3'-O3'	6.84	135.18	112.60
1	D	1	DG	O4'-C4'-C3'	6.83	110.10	106.00
1	D	6	DT	N3-C4-C5	6.79	119.27	115.20
2	A	512	THR	CB-CA-C	-6.78	93.30	111.60
2	A	488	ARG	NE-CZ-NH2	6.78	123.69	120.30
1	D	8	DT	O5'-C5'-C4'	-6.74	94.15	111.00
1	C	-4	DC	O5'-C5'-C4'	-6.72	94.19	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	-9	DC	C5'-C4'-O4'	6.66	121.94	109.30
1	D	-7	DG	N9-C1'-C2'	6.65	125.23	112.60
1	C	-3	DA	N9-C1'-C2'	-6.63	100.01	112.60
1	C	-1	DC	O4'-C4'-C3'	6.62	109.97	106.00
1	D	4	DG	C5-C6-N1	6.60	114.80	111.50
1	C	-7	DG	C5-C6-N1	6.56	114.78	111.50
2	B	485	ASP	CB-CG-OD2	-6.54	112.41	118.30
2	A	456	THR	N-CA-CB	-6.54	97.87	110.30
1	D	9	DG	C6-N1-C2	-6.53	121.18	125.10
2	A	498	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	C	1	DG	N1-C2-N2	-6.51	110.34	116.20
1	C	7	DC	O5'-P-OP1	6.51	118.51	110.70
1	C	-9	DC	OP1-P-O3'	-6.50	90.89	105.20
1	C	3	DT	C2-N3-C4	-6.49	123.31	127.20
2	A	489	ARG	NE-CZ-NH2	6.48	123.54	120.30
1	D	1	DG	C5'-C4'-O4'	-6.47	97.01	109.30
1	C	4	DG	N1-C2-N3	6.46	127.78	123.90
1	D	-1	DC	P-O3'-C3'	6.45	127.44	119.70
1	D	1	DG	OP1-P-OP2	-6.45	109.93	119.60
2	B	488	ARG	NE-CZ-NH2	6.42	123.51	120.30
1	C	9	DG	C5-C6-O6	-6.39	124.77	128.60
2	B	480	ASN	CA-CB-CG	-6.39	99.34	113.40
1	C	-7	DG	C6-N1-C2	-6.38	121.27	125.10
1	D	-7	DG	N1-C2-N3	6.38	127.73	123.90
1	D	-5	DA	N1-C2-N3	-6.38	126.11	129.30
1	C	6	DT	N3-C4-C5	6.37	119.02	115.20
2	B	496	ARG	CD-NE-CZ	-6.35	114.71	123.60
2	B	434	MET	CG-SD-CE	6.35	110.36	100.20
1	C	2	DA	P-O3'-C3'	-6.35	112.08	119.70
2	B	446	GLU	CG-CD-OE1	-6.30	105.69	118.30
1	D	-8	DA	O3'-P-O5'	-6.29	92.04	104.00
1	D	-4	DC	N1-C1'-C2'	-6.29	100.65	112.60
1	D	5	DT	C6-C5-C7	-6.28	119.13	122.90
1	C	-1	DC	C5'-C4'-O4'	6.28	121.23	109.30
1	D	-7	DG	OP1-P-OP2	-6.28	110.19	119.60
1	C	2	DA	C5-C6-N1	-6.27	114.56	117.70
1	D	7	DC	C5'-C4'-O4'	6.27	121.21	109.30
2	B	489	ARG	CD-NE-CZ	-6.26	114.83	123.60
1	C	-1	DC	O5'-C5'-C4'	-6.26	95.36	111.00
1	C	1	DG	O4'-C1'-N9	-6.24	103.63	108.00
1	D	-7	DG	C5-N7-C8	-6.24	101.18	104.30
1	D	-2	DT	P-O3'-C3'	-6.23	112.22	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	4	DG	C6-N1-C2	-6.20	121.38	125.10
1	C	3	DT	P-O5'-C5'	-6.17	111.02	120.90
1	C	7	DC	O4'-C1'-C2'	-6.17	100.96	105.90
1	D	2	DA	O4'-C1'-C2'	-6.15	100.98	105.90
2	B	482	CYS	CA-C-O	-6.14	107.21	120.10
1	D	-2	DT	C5'-C4'-O4'	6.13	120.94	109.30
1	D	-7	DG	N1-C2-N2	-6.12	110.69	116.20
2	B	489	ARG	CA-CB-CG	6.08	126.78	113.40
1	C	1	DG	N1-C2-N3	6.06	127.54	123.90
1	D	-8	DA	C2-N3-C4	6.06	113.63	110.60
2	A	498	ARG	NE-CZ-NH2	6.05	123.33	120.30
2	B	451	HIS	CB-CA-C	6.03	122.46	110.40
2	B	505	MET	CG-SD-CE	6.03	109.84	100.20
1	D	-7	DG	OP2-P-O3'	6.02	118.44	105.20
2	A	485	ASP	CB-CA-C	6.02	122.44	110.40
1	D	-3	DA	C6-N1-C2	6.01	122.21	118.60
1	D	7	DC	O3'-P-O5'	-6.00	92.59	104.00
1	D	9	DG	C8-N9-C1'	6.00	134.81	127.00
1	C	-3	DA	C4-C5-C6	5.96	119.98	117.00
1	C	-10	DC	N1-C2-O2	5.92	122.45	118.90
2	A	446	GLU	CG-CD-OE2	5.89	130.09	118.30
1	D	1	DG	O3'-P-O5'	-5.89	92.80	104.00
1	C	3	DT	N3-C4-C5	5.88	118.73	115.20
1	D	-9	DC	C5'-C4'-C3'	5.87	124.67	114.10
1	C	7	DC	C5-C6-N1	5.86	123.93	121.00
2	A	462	VAL	O-C-N	5.85	132.06	122.70
1	D	-2	DT	N3-C4-C5	5.85	118.71	115.20
2	A	505	MET	CG-SD-CE	5.84	109.54	100.20
2	B	459	SER	N-CA-CB	5.83	119.24	110.50
1	D	5	DT	P-O3'-C3'	5.81	126.67	119.70
1	D	-4	DC	P-O3'-C3'	-5.81	112.73	119.70
2	B	498	ARG	NH1-CZ-NH2	-5.80	113.02	119.40
1	C	5	DT	P-O5'-C5'	-5.80	111.63	120.90
2	B	513	LYS	N-CA-CB	5.79	121.03	110.60
2	B	442	VAL	O-C-N	-5.78	113.45	122.70
1	C	-1	DC	O3'-P-O5'	-5.77	93.03	104.00
1	D	-5	DA	O5'-P-OP2	-5.76	100.52	105.70
2	B	481	ASP	CB-CG-OD1	-5.74	113.13	118.30
2	A	471	GLN	N-CA-CB	5.74	120.93	110.60
2	A	498	ARG	NH1-CZ-NH2	-5.72	113.11	119.40
1	C	-6	DA	C2-N3-C4	5.71	113.45	110.60
1	D	5	DT	C4-C5-C7	5.71	122.42	119.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1	DG	C4-N9-C1'	5.69	133.90	126.50
1	D	-2	DT	N1-C2-N3	5.69	118.01	114.60
1	D	4	DG	C5-C6-O6	5.67	132.00	128.60
1	C	-6	DA	OP1-P-OP2	-5.67	111.10	119.60
1	C	-2	DT	N3-C2-O2	-5.66	118.91	122.30
1	C	-9	DC	N3-C4-C5	5.65	124.16	121.90
1	D	5	DT	N3-C4-O4	-5.65	116.51	119.90
2	A	437	ALA	O-C-N	-5.65	113.67	122.70
1	D	-1	DC	N1-C2-O2	5.64	122.28	118.90
2	A	434	MET	CB-CA-C	-5.64	99.12	110.40
1	C	9	DG	N3-C2-N2	-5.63	115.96	119.90
1	C	1	DG	C8-N9-C1'	-5.60	119.72	127.00
1	C	9	DG	N1-C2-N3	5.59	127.25	123.90
1	C	-7	DG	C5'-C4'-O4'	5.58	119.91	109.30
1	C	-3	DA	N1-C6-N6	5.58	121.94	118.60
1	D	9	DG	C8-N9-C4	-5.57	104.17	106.40
1	C	-2	DT	P-O5'-C5'	-5.54	112.04	120.90
2	B	480	ASN	CB-CG-OD1	-5.54	110.53	121.60
1	D	-1	DC	C6-N1-C2	-5.53	118.09	120.30
1	C	-4	DC	P-O5'-C5'	-5.51	112.08	120.90
1	C	1	DG	C5-C6-N1	5.51	114.25	111.50
1	D	2	DA	C5-C6-N1	-5.51	114.95	117.70
1	C	-9	DC	N1-C2-O2	5.50	122.20	118.90
1	D	9	DG	N1-C6-O6	-5.50	116.60	119.90
1	D	4	DG	C6-C5-N7	5.48	133.69	130.40
1	C	-6	DA	C6-N1-C2	5.47	121.88	118.60
1	C	-3	DA	C6-C5-N7	-5.47	128.47	132.30
2	A	454	VAL	N-CA-CB	-5.46	99.49	111.50
2	B	510	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	D	7	DC	C6-N1-C2	5.42	122.47	120.30
2	A	479	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	C	7	DC	O4'-C1'-N1	5.40	111.78	108.00
1	D	-1	DC	OP1-P-OP2	-5.37	111.55	119.60
1	C	-2	DT	OP1-P-O3'	5.36	116.99	105.20
1	C	5	DT	N3-C2-O2	-5.36	119.08	122.30
1	D	6	DT	O5'-C5'-C4'	-5.35	97.63	111.00
1	C	-8	DA	O4'-C1'-C2'	-5.34	101.63	105.90
1	C	-1	DC	O4'-C1'-C2'	-5.34	101.63	105.90
1	D	5	DT	O3'-P-O5'	-5.33	93.86	104.00
2	B	466	ARG	NE-CZ-NH1	5.33	122.96	120.30
2	A	466	ARG	NE-CZ-NH1	5.32	122.96	120.30
2	B	445	ASP	CB-CG-OD1	-5.31	113.52	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	8	DT	C5-C4-O4	-5.30	121.19	124.90
1	D	9	DG	C4-N9-C1'	-5.30	119.61	126.50
1	D	-10	DC	C4'-C3'-O3'	5.30	122.94	109.70
1	D	3	DT	O5'-P-OP1	-5.28	100.95	105.70
1	C	9	DG	O4'-C4'-C3'	5.24	109.14	106.00
1	D	-7	DG	O4'-C1'-C2'	-5.20	101.74	105.90
1	C	-6	DA	C5-C6-N1	-5.19	115.10	117.70
2	B	498	ARG	NE-CZ-NH2	5.17	122.89	120.30
1	C	-5	DA	C5-C6-N1	-5.15	115.13	117.70
2	B	445	ASP	CB-CG-OD2	5.15	122.93	118.30
1	D	3	DT	N1-C1'-C2'	5.14	122.36	112.60
1	D	3	DT	OP1-P-OP2	5.10	127.26	119.60
1	C	5	DT	O5'-P-OP1	5.10	116.82	110.70
1	C	-9	DC	O3'-P-O5'	5.09	113.67	104.00
2	B	488	ARG	NH1-CZ-NH2	-5.08	113.81	119.40
1	C	-3	DA	C8-N9-C1'	-5.07	118.58	127.70
1	D	7	DC	OP1-P-OP2	-5.06	112.00	119.60
2	A	437	ALA	CB-CA-C	-5.06	102.50	110.10
2	B	498	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	C	-5	DA	O3'-P-O5'	-5.05	94.41	104.00
1	C	-3	DA	P-O5'-C5'	-5.05	112.82	120.90
2	A	446	GLU	OE1-CD-OE2	-5.05	117.24	123.30
1	C	-6	DA	O4'-C1'-C2'	-5.04	101.87	105.90
1	D	-7	DG	O5'-C5'-C4'	-5.04	98.41	111.00
1	D	2	DA	N7-C8-N9	-5.03	111.28	113.80
1	D	4	DG	N9-C4-C5	5.03	107.41	105.40
1	C	9	DG	C5'-C4'-O4'	5.03	118.86	109.30
1	C	-7	DG	OP2-P-O3'	5.01	116.22	105.20

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	435	LYS	Mainchain,Peptide
2	A	437	ALA	Mainchain
2	A	439	PRO	Mainchain
2	A	451	HIS	Mainchain
2	A	453	GLY	Mainchain
2	A	466	ARG	Sidechain
2	A	476	CYS	Mainchain
2	A	497	TYR	Mainchain
2	A	504	GLY	Mainchain

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Mol	Chain	Res	Type	Group
2	B	442	VAL	Mainchain
2	B	450	CYS	Mainchain
2	B	455	LEU	Mainchain
2	B	466	ARG	Sidechain
2	B	488	ARG	Sidechain
2	B	498	ARG	Sidechain
1	C	-3	DA	Sidechain
1	C	3	DT	Sidechain
1	D	-8	DA	Sidechain
1	D	6	DT	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	C	385	0	216	28	0
1	D	385	0	216	32	0
2	A	628	0	635	116	0
2	B	628	0	637	73	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	7	0	0	2	0
4	B	18	0	0	4	0
4	C	7	0	0	1	0
4	D	9	0	0	3	0
All	All	2071	0	1704	228	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 62.

All (228) 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:A:437:ALA:O	2:A:439:PRO:HD2	1.15	1.29
2:A:450:CYS:SG	2:A:513:LYS:HG2	1.70	1.29
2:A:437:ALA:O	2:A:439:PRO:CD	1.85	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:475:LEU:HD23	2:B:488:ARG:NH1	1.61	1.15
2:A:446:GLU:O	2:A:446:GLU:HG2	1.42	1.14
2:A:434:MET:HG2	2:A:436:PRO:HD3	1.29	1.13
2:A:438:ARG:HB2	2:A:439:PRO:HD3	1.13	1.13
2:A:475:LEU:HD23	2:B:488:ARG:HH12	1.11	1.12
1:D:-4:DC:H2''	1:D:-3:DA:H5'	1.07	1.06
2:A:475:LEU:CD2	2:B:488:ARG:NH1	2.18	1.06
1:C:-1:DC:H2''	1:C:1:DG:C8	1.90	1.06
2:A:451:HIS:HB3	2:A:461:LYS:HG2	1.36	1.04
2:A:512:THR:HG22	2:A:513:LYS:N	1.69	1.03
1:D:-4:DC:C2'	1:D:-3:DA:H5'	1.88	1.02
1:D:-10:DC:H2''	1:D:-9:DC:C6	1.96	1.01
1:D:-10:DC:H4'	2:A:514:LYS:HB2	1.43	1.01
1:D:-4:DC:H2''	1:D:-3:DA:C5'	1.94	0.97
2:A:436:PRO:O	2:A:455:LEU:HD22	1.64	0.97
2:A:438:ARG:HB2	2:A:439:PRO:CD	1.95	0.96
2:A:450:CYS:SG	2:A:513:LYS:CG	2.53	0.95
2:A:512:THR:CG2	2:A:513:LYS:N	2.28	0.95
2:A:438:ARG:CB	2:A:439:PRO:HD3	1.97	0.95
2:B:442:VAL:CG2	2:B:442:VAL:O	2.16	0.93
2:B:462:VAL:HG23	4:B:12:HOH:O	1.66	0.93
2:A:475:LEU:CD2	2:B:488:ARG:HH12	1.78	0.91
1:D:-4:DC:OP1	1:D:-4:DC:H4'	1.71	0.91
2:A:450:CYS:HB2	2:A:513:LYS:HB2	1.52	0.90
2:B:473:ASN:C	2:B:473:ASN:HD22	1.76	0.88
2:B:442:VAL:O	2:B:442:VAL:HG22	1.72	0.88
2:A:512:THR:HG22	2:A:513:LYS:CA	2.05	0.86
2:A:434:MET:CG	2:A:436:PRO:HD3	2.05	0.85
1:C:-3:DA:H1'	1:C:-2:DT:O5'	1.78	0.83
1:C:8:DT:O4	4:C:13:HOH:O	1.96	0.83
2:A:434:MET:HG2	2:A:436:PRO:CD	2.08	0.82
2:A:506:ASN:HB3	2:A:509:ALA:HB2	1.61	0.82
2:B:452:TYR:OH	2:B:465:LYS:HG3	1.81	0.79
1:C:-1:DC:C2'	1:C:1:DG:C8	2.66	0.79
2:A:436:PRO:O	2:A:455:LEU:CD2	2.31	0.79
1:C:-4:DC:H5''	1:C:-4:DC:H6	1.45	0.79
2:A:434:MET:CG	2:A:435:LYS:H	1.96	0.77
2:A:434:MET:O	2:A:435:LYS:HG3	1.84	0.77
2:A:512:THR:HG22	2:A:513:LYS:HA	1.65	0.77
2:B:456:THR:HG21	2:B:505:MET:CE	2.15	0.77
1:D:8:DT:H2'	1:D:9:DG:C8	2.21	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:483:ILE:O	2:A:483:ILE:HG22	1.85	0.75
2:A:437:ALA:O	2:A:439:PRO:N	2.19	0.74
2:A:434:MET:HG2	2:A:435:LYS:N	2.02	0.74
2:A:434:MET:CG	2:A:435:LYS:N	2.46	0.74
2:A:457:CYS:O	2:A:461:LYS:HB2	1.88	0.74
2:A:459:SER:OG	2:A:460:CYS:N	2.17	0.73
2:A:434:MET:HG2	2:A:435:LYS:H	1.52	0.73
2:A:495:CYS:O	2:A:498:ARG:HG2	1.86	0.73
2:B:473:ASN:ND2	2:B:473:ASN:C	2.40	0.73
2:A:475:LEU:HD22	2:B:488:ARG:NH1	2.02	0.72
1:C:-3:DA:H4'	1:C:-2:DT:OP1	1.88	0.72
2:B:487:ILE:CG1	4:B:37:HOH:O	2.36	0.72
2:B:487:ILE:HG12	4:B:37:HOH:O	1.88	0.72
2:B:512:THR:O	2:B:513:LYS:C	2.27	0.72
2:A:514:LYS:C	2:A:514:LYS:HD3	2.09	0.71
2:B:463:PHE:CD2	2:B:496:ARG:HD3	2.26	0.70
2:A:482:CYS:HB3	2:B:477:ALA:HB1	1.74	0.70
2:A:465:LYS:NZ	2:A:469:GLU:OE2	2.25	0.70
2:A:446:GLU:O	2:A:446:GLU:CG	2.27	0.69
2:B:458:GLY:O	2:B:461:LYS:HB3	1.92	0.69
2:B:484:ILE:O	2:B:485:ASP:HB3	1.92	0.68
2:A:512:THR:O	2:A:513:LYS:HB2	1.92	0.68
1:C:-4:DC:H2''	1:C:-3:DA:C8	2.28	0.68
2:A:498:ARG:HG3	2:A:499:LYS:N	2.08	0.67
2:A:451:HIS:CB	2:A:461:LYS:HG2	2.17	0.67
2:B:484:ILE:HD13	2:B:499:LYS:HD3	1.77	0.65
2:B:473:ASN:HD22	2:B:474:TYR:N	1.94	0.65
2:A:482:CYS:HB3	2:B:477:ALA:CB	2.26	0.65
2:A:463:PHE:CE1	2:A:496:ARG:HD3	2.31	0.65
1:D:-10:DC:H2''	1:D:-9:DC:H6	1.54	0.65
2:A:459:SER:CB	2:A:489:ARG:NH1	2.60	0.64
2:B:510:ARG:NH1	2:B:513:LYS:HE3	2.13	0.64
2:A:457:CYS:SG	2:A:459:SER:OG	2.56	0.64
1:C:-5:DA:H2''	1:C:-4:DC:O5'	1.98	0.64
2:B:484:ILE:O	2:B:485:ASP:CB	2.47	0.63
1:D:8:DT:H2''	1:D:9:DG:O4'	1.98	0.63
1:D:-6:DA:H2''	1:D:-5:DA:C8	2.35	0.62
2:A:488:ARG:HD3	2:B:477:ALA:HA	1.81	0.62
2:A:483:ILE:HD13	2:A:488:ARG:NH1	2.15	0.61
2:A:434:MET:O	2:A:435:LYS:CB	2.47	0.61
2:A:434:MET:O	2:A:435:LYS:CG	2.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:-8:DA:OP2	2:B:451:HIS:HD2	1.84	0.60
2:B:488:ARG:O	2:B:491:ASN:HB2	2.02	0.60
2:A:459:SER:HB3	2:A:489:ARG:HH12	1.66	0.60
2:B:440:CYS:SG	2:B:456:THR:HA	2.41	0.60
2:A:462:VAL:HG12	2:A:466:ARG:HE	1.65	0.60
1:C:5:DT:H71	2:A:462:VAL:CG2	2.31	0.59
1:D:4:DG:H2''	1:D:5:DT:C5'	2.33	0.59
2:A:485:ASP:O	2:A:487:ILE:N	2.36	0.59
1:C:-3:DA:C1'	1:C:-2:DT:O5'	2.49	0.59
1:D:-4:DC:H6	1:D:-4:DC:H5''	1.67	0.58
2:A:452:TYR:HE2	2:A:461:LYS:HD3	1.68	0.58
2:B:484:ILE:CG2	2:B:485:ASP:N	2.66	0.58
2:B:442:VAL:HG23	2:B:442:VAL:O	2.03	0.58
2:B:447:ALA:CB	2:B:455:LEU:HD13	2.34	0.58
2:A:443:CYS:SG	2:A:443:CYS:O	2.62	0.57
2:B:483:ILE:O	2:B:484:ILE:HG13	2.04	0.57
1:D:-4:DC:H1'	4:D:16:HOH:O	2.04	0.57
2:B:440:CYS:SG	2:B:441:LEU:N	2.77	0.57
2:A:450:CYS:HB2	2:A:513:LYS:CB	2.31	0.57
2:A:485:ASP:O	2:A:486:LYS:C	2.41	0.57
2:A:452:TYR:CD1	2:A:507:LEU:HD12	2.40	0.57
2:B:448:SER:OG	2:B:451:HIS:HE1	1.88	0.57
2:A:504:GLY:O	2:A:505:MET:C	2.43	0.56
2:B:512:THR:O	2:B:513:LYS:O	2.23	0.56
1:D:4:DG:H2''	1:D:5:DT:H5'	1.87	0.56
2:A:513:LYS:O	2:A:514:LYS:C	2.43	0.56
2:A:463:PHE:CE1	2:A:496:ARG:HB3	2.41	0.56
2:A:500:CYS:O	2:A:501:LEU:C	2.45	0.55
2:B:485:ASP:O	2:B:487:ILE:N	2.40	0.55
2:A:458:GLY:O	2:A:462:VAL:HG23	2.06	0.55
2:A:481:ASP:CG	2:B:479:ARG:HH22	2.10	0.55
2:B:443:CYS:HA	2:B:484:ILE:CG2	2.37	0.54
2:A:506:ASN:OD1	2:A:507:LEU:N	2.41	0.54
2:A:488:ARG:O	2:A:491:ASN:HB2	2.08	0.53
2:A:451:HIS:O	2:A:453:GLY:N	2.41	0.53
1:D:-10:DC:H2''	1:D:-9:DC:C5	2.40	0.53
2:A:476:CYS:HB2	2:A:492:CYS:SG	2.48	0.53
2:B:462:VAL:O	2:B:462:VAL:HG22	2.08	0.53
2:B:459:SER:OG	2:B:489:ARG:NH2	2.42	0.53
1:C:-4:DC:C6	1:C:-4:DC:H5''	2.36	0.52
2:A:456:THR:HG23	2:A:457:CYS:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:-4:DC:H2''	1:C:-3:DA:O5'	2.08	0.52
1:D:-4:DC:C1'	4:D:16:HOH:O	2.56	0.52
2:A:434:MET:SD	2:A:436:PRO:HD3	2.50	0.52
1:C:-4:DC:H2''	1:C:-3:DA:H8	1.72	0.52
2:A:484:ILE:O	2:A:485:ASP:HB3	2.10	0.52
1:D:-7:DG:H5''	4:D:17:HOH:O	2.10	0.52
2:A:475:LEU:HD22	2:B:488:ARG:CZ	2.39	0.52
2:B:451:HIS:O	2:B:452:TYR:C	2.48	0.51
1:C:-3:DA:O5'	1:C:-3:DA:H2'	2.10	0.51
2:A:440:CYS:HB3	2:A:445:ASP:H	1.75	0.50
2:A:459:SER:HB2	2:A:489:ARG:NH1	2.26	0.50
1:C:5:DT:H71	2:A:462:VAL:HG21	1.92	0.50
2:B:443:CYS:HA	2:B:484:ILE:HG22	1.93	0.50
2:A:514:LYS:C	2:A:514:LYS:CD	2.78	0.50
1:C:4:DG:C2	1:D:-3:DA:C2	3.00	0.50
2:B:462:VAL:O	2:B:462:VAL:CG2	2.59	0.50
1:D:-2:DT:H2''	1:D:-1:DC:O5'	2.11	0.50
2:A:436:PRO:O	2:A:437:ALA:HB3	2.12	0.50
2:A:498:ARG:CG	2:A:499:LYS:N	2.74	0.50
2:B:465:LYS:NZ	2:B:469:GLU:OE1	2.35	0.49
2:B:487:ILE:HG13	4:B:37:HOH:O	2.06	0.49
2:A:458:GLY:O	2:A:461:LYS:HB3	2.13	0.49
2:A:437:ALA:O	2:A:438:ARG:C	2.50	0.49
2:A:459:SER:CB	2:A:489:ARG:HH12	2.22	0.49
2:A:452:TYR:CE2	2:A:461:LYS:HD3	2.48	0.49
1:D:5:DT:H2'	1:D:5:DT:O5'	2.13	0.48
1:D:-7:DG:H2''	1:D:-6:DA:C8	2.47	0.48
2:A:461:LYS:NZ	4:A:19:HOH:O	2.47	0.48
2:B:456:THR:HG21	2:B:505:MET:HE1	1.92	0.48
2:B:512:THR:O	2:B:514:LYS:O	2.31	0.48
2:A:473:ASN:ND2	4:A:30:HOH:O	2.46	0.48
1:C:-5:DA:C2'	1:C:-4:DC:O5'	2.60	0.48
2:B:507:LEU:HA	2:B:507:LEU:HD22	1.47	0.48
2:A:481:ASP:OD2	2:B:479:ARG:NH2	2.42	0.47
2:A:482:CYS:HB3	2:B:477:ALA:O	2.14	0.47
2:B:440:CYS:SG	2:B:442:VAL:HG13	2.54	0.47
2:B:456:THR:HG21	2:B:505:MET:HE3	1.96	0.47
2:A:434:MET:O	2:A:435:LYS:HB2	2.15	0.46
2:A:459:SER:HB2	2:A:496:ARG:HH22	1.79	0.46
2:A:475:LEU:HD13	2:B:487:ILE:HD12	1.96	0.46
2:A:456:THR:CG2	2:A:457:CYS:N	2.77	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:463:PHE:CD1	2:A:496:ARG:HD3	2.50	0.46
2:B:484:ILE:HG22	2:B:485:ASP:N	2.31	0.46
1:D:-7:DG:H2''	1:D:-6:DA:H8	1.80	0.46
1:C:-6:DA:H2''	1:C:-5:DA:C8	2.51	0.46
1:D:3:DT:C2'	1:D:4:DG:OP2	2.64	0.46
2:A:492:CYS:HB3	2:A:495:CYS:HB2	1.98	0.45
2:B:485:ASP:O	2:B:486:LYS:C	2.54	0.45
1:D:-10:DC:O5'	1:D:-10:DC:H2'	2.15	0.45
2:A:442:VAL:C	2:A:499:LYS:HZ2	2.19	0.45
2:B:447:ALA:HB1	2:B:455:LEU:HD13	1.98	0.45
2:B:492:CYS:HA	2:B:493:PRO:HD2	1.92	0.45
2:A:482:CYS:CB	2:B:477:ALA:HB1	2.44	0.45
2:A:442:VAL:C	2:A:499:LYS:NZ	2.70	0.44
2:A:451:HIS:HB3	2:A:461:LYS:CG	2.26	0.44
1:C:-3:DA:O5'	1:C:-3:DA:C2'	2.66	0.44
1:D:-8:DA:H2''	1:D:-7:DG:O5'	2.16	0.44
2:B:485:ASP:OD1	2:B:488:ARG:HG3	2.17	0.44
2:A:436:PRO:O	2:A:437:ALA:CB	2.66	0.44
2:A:451:HIS:CG	2:A:461:LYS:HG3	2.52	0.44
2:B:490:LYS:H	2:B:490:LYS:HG3	1.65	0.44
2:A:496:ARG:O	2:A:499:LYS:N	2.51	0.44
2:B:451:HIS:O	2:B:453:GLY:N	2.51	0.44
2:B:441:LEU:HB2	2:B:454:VAL:CG1	2.48	0.44
2:A:506:ASN:CB	2:A:509:ALA:HB2	2.41	0.43
1:D:4:DG:H2''	1:D:5:DT:O5'	2.19	0.43
2:B:510:ARG:CZ	2:B:513:LYS:HE3	2.48	0.43
2:B:474:TYR:HB2	2:B:494:ALA:HB2	2.00	0.43
1:D:3:DT:H2''	1:D:4:DG:OP2	2.18	0.43
1:C:-4:DC:C2'	1:C:-3:DA:C8	3.00	0.43
2:A:500:CYS:O	2:A:502:GLN:N	2.52	0.43
2:A:451:HIS:CB	2:A:461:LYS:CG	2.94	0.43
2:B:463:PHE:CE2	2:B:496:ARG:HD3	2.54	0.43
1:C:4:DG:N7	2:A:466:ARG:NH2	2.66	0.42
2:A:438:ARG:CB	2:A:439:PRO:CD	2.66	0.42
2:A:506:ASN:HB3	2:A:509:ALA:CB	2.42	0.42
2:B:459:SER:O	2:B:460:CYS:C	2.58	0.42
2:A:488:ARG:O	2:A:491:ASN:N	2.43	0.42
2:A:507:LEU:HA	2:A:507:LEU:HD12	1.40	0.42
2:A:449:GLY:O	2:A:451:HIS:N	2.52	0.42
2:B:448:SER:OG	2:B:451:HIS:CE1	2.71	0.42
2:B:512:THR:C	2:B:513:LYS:O	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:-10:DC:H2''	1:C:-9:DC:C6	2.54	0.42
1:D:-4:DC:OP1	1:D:-4:DC:C4'	2.53	0.42
2:B:501:LEU:HA	2:B:501:LEU:HD12	1.85	0.42
2:B:504:GLY:O	2:B:505:MET:C	2.57	0.41
1:C:-6:DA:C2'	1:C:-5:DA:C8	3.04	0.41
1:D:-10:DC:H4'	2:A:514:LYS:CB	2.30	0.41
1:D:-4:DC:H6	1:D:-4:DC:C5'	2.33	0.41
2:A:465:LYS:NZ	2:A:469:GLU:CD	2.73	0.41
2:A:497:TYR:O	2:A:498:ARG:C	2.57	0.41
2:A:508:GLU:OE1	2:A:508:GLU:O	2.37	0.41
1:C:-6:DA:H2''	1:C:-5:DA:O4'	2.20	0.41
2:B:441:LEU:HD22	2:B:441:LEU:HA	1.86	0.41
1:C:-7:DG:H2''	1:C:-6:DA:OP2	2.20	0.41
1:D:6:DT:H2'	1:D:6:DT:H6	1.67	0.41
1:C:-3:DA:H1'	1:C:-2:DT:C5'	2.51	0.41
2:B:508:GLU:OE1	2:B:511:LYS:HG3	2.20	0.40
1:D:5:DT:C2'	1:D:5:DT:O5'	2.68	0.40
2:A:451:HIS:CG	2:A:461:LYS:CG	3.05	0.40
1:C:-3:DA:OP2	1:C:-3:DA:H3'	2.22	0.40
2:A:450:CYS:CB	2:A:513:LYS:HB2	2.36	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	
2	A	79/81 (98%)	51 (65%)	18 (23%)	10 (13%)	0	0
2	B	79/81 (98%)	58 (73%)	15 (19%)	6 (8%)	1	2
All	All	158/162 (98%)	109 (69%)	33 (21%)	16 (10%)	0	1

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	436	PRO
2	A	437	ALA
2	A	438	ARG
2	A	452	TYR
2	A	500	CYS
2	A	513	LYS
2	B	436	PRO
2	B	513	LYS
2	A	501	LEU
2	B	486	LYS
2	A	444	SER
2	A	450	CYS
2	B	452	TYR
2	B	471	GLN
2	B	485	ASP
2	A	459	SER

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	
2	A	68/68 (100%)	47 (69%)	21 (31%)	0	1
2	B	68/68 (100%)	52 (76%)	16 (24%)	1	2
All	All	136/136 (100%)	99 (73%)	37 (27%)	0	1

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	441	LEU
2	A	443	CYS
2	A	444	SER
2	A	446	GLU
2	A	450	CYS
2	A	456	THR
2	A	461	LYS
2	A	462	VAL

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Mol	Chain	Res	Type
2	A	471	GLN
2	A	476	CYS
2	A	479	ARG
2	A	480	ASN
2	A	482	CYS
2	A	485	ASP
2	A	487	ILE
2	A	490	LYS
2	A	501	LEU
2	A	508	GLU
2	A	510	ARG
2	A	513	LYS
2	A	514	LYS
2	B	434	MET
2	B	438	ARG
2	B	440	CYS
2	B	441	LEU
2	B	442	VAL
2	B	450	CYS
2	B	473	ASN
2	B	479	ARG
2	B	486	LYS
2	B	490	LYS
2	B	498	ARG
2	B	501	LEU
2	B	506	ASN
2	B	507	LEU
2	B	512	THR
2	B	513	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	473	ASN
2	A	491	ASN
2	B	451	HIS
2	B	473	ASN
2	B	506	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 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 ⓘ

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.