Full wwPDB X-ray Structure Validation Report ⓘ

Aug 14, 2023 – 01:17 PM EDT

PDB ID	:	1R4O
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	:	2003-10-07
Resolution	:	2.50 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:

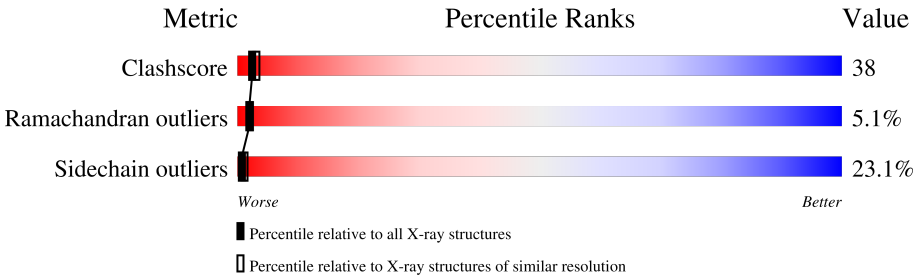
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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 <=5%

Mol	Chain	Length	Quality of chain
1	C	19	21% 68% 11%
1	D	19	32% 58% 11%
2	A	92	33% 27% 17% 10% 13%
2	B	92	25% 30% 23% 9% 13%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 2121 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 5'-D(*CP*CP*AP*GP*AP*AP*CP*AP*TP*CP*GP*AP*TP*GP*TP*TP*CP*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 Glucocorticoid receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	80	Total	C	N	O	S	0	0	0
			619	379	122	106	12			
2	B	80	Total	C	N	O	S	0	0	0
			619	379	122	106	12			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	434	MET	-	cloning artifact	UNP P06536
A	435	LYS	-	cloning artifact	UNP P06536
A	436	PRO	-	cloning artifact	UNP P06536
A	437	ALA	-	cloning artifact	UNP P06536
A	438	ARG	-	cloning artifact	UNP P06536
A	439	PRO	-	cloning artifact	UNP P06536
B	434	MET	-	cloning artifact	UNP P06536
B	435	LYS	-	cloning artifact	UNP P06536
B	436	PRO	-	cloning artifact	UNP P06536
B	437	ALA	-	cloning artifact	UNP P06536
B	438	ARG	-	cloning artifact	UNP P06536
B	439	PRO	-	cloning artifact	UNP P06536

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

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	23	Total O 23 23	0	0
4	D	13	Total O 13 13	0	0
4	A	32	Total O 32 32	0	0
4	B	41	Total O 41 41	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. 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.

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

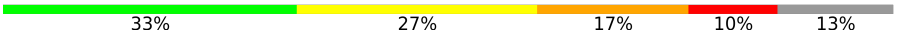
Chain C:

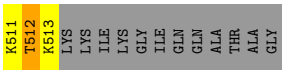
• Molecule 1: 5'-D(*CP*CP*AP*GP*AP*AP*CP*AP*TP*CP*GP*AP*TP*GP*TP*TP*CP*TP*G)-3'

Chain D:

• Molecule 2: Glucocorticoid receptor

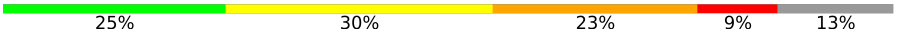
Chain A:





• Molecule 2: Glucocorticoid receptor

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	38.50Å 97.50Å 120.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.50 19.67 – 2.48	Depositor EDS
% Data completeness (in resolution range)	(Not available) (6.00-2.50) 84.9 (19.67-2.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	7.78 (at 2.46Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.196 , (Not available) 0.274 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	44.8	Xtriage
Anisotropy	0.528	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 73.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	2121	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.88% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	2.55	25/431 (5.8%)	4.77	147/663 (22.2%)
1	D	2.62	29/431 (6.7%)	4.72	145/663 (21.9%)
2	A	0.97	0/628	2.46	34/837 (4.1%)
2	B	1.13	0/628	3.06	45/837 (5.4%)
All	All	1.84	54/2118 (2.5%)	3.77	371/3000 (12.4%)

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	4
2	A	0	8
2	B	0	13
All	All	0	27

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	5	DA	P-O5'	11.99	1.71	1.59
1	D	2	DC	O3'-P	10.45	1.73	1.61
1	C	17	DC	O3'-P	10.15	1.73	1.61
1	C	8	DA	P-O5'	9.79	1.69	1.59
1	C	6	DA	O3'-P	9.57	1.72	1.61
1	C	6	DA	P-O5'	8.83	1.68	1.59
1	D	10	DC	O3'-P	8.71	1.71	1.61
1	C	2	DC	P-O5'	-8.52	1.51	1.59
1	D	17	DC	O3'-P	8.38	1.71	1.61
1	D	17	DC	O4'-C1'	8.14	1.52	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1	DC	C4'-O4'	-7.86	1.37	1.45
1	C	11	DG	C8-N7	7.78	1.35	1.30
1	D	14	DG	O3'-P	-7.76	1.51	1.61
1	D	9	DT	P-O5'	7.53	1.67	1.59
1	D	11	DG	P-O5'	7.43	1.67	1.59
1	C	8	DA	O3'-P	7.29	1.69	1.61
1	C	2	DC	P-OP2	7.17	1.61	1.49
1	D	8	DA	O3'-P	-7.17	1.52	1.61
1	D	17	DC	P-OP1	6.96	1.60	1.49
1	D	12	DA	P-O5'	6.66	1.66	1.59
1	D	9	DT	C4-O4	6.60	1.29	1.23
1	C	9	DT	C4-O4	6.53	1.29	1.23
1	D	4	DG	O3'-P	6.43	1.68	1.61
1	C	19	DG	P-O5'	-6.36	1.53	1.59
1	C	9	DT	P-OP2	6.34	1.59	1.49
1	D	7	DC	P-O5'	6.34	1.66	1.59
1	D	3	DA	C4'-O4'	-6.31	1.38	1.45
1	D	1	DC	O3'-P	6.18	1.68	1.61
1	C	10	DC	O3'-P	6.04	1.68	1.61
1	C	2	DC	O4'-C1'	6.01	1.49	1.42
1	D	12	DA	N1-C2	6.00	1.39	1.34
1	D	15	DT	P-O5'	5.96	1.65	1.59
1	D	9	DT	C4'-O4'	-5.95	1.39	1.45
1	C	4	DG	C8-N7	5.71	1.34	1.30
1	D	7	DC	O3'-P	5.71	1.68	1.61
1	C	17	DC	P-O5'	5.68	1.65	1.59
1	C	15	DT	O3'-P	5.64	1.68	1.61
1	D	13	DT	C4-O4	5.64	1.28	1.23
1	D	2	DC	P-O5'	-5.63	1.54	1.59
1	D	16	DT	O3'-P	5.60	1.67	1.61
1	D	19	DG	N7-C5	5.54	1.42	1.39
1	C	14	DG	P-O5'	5.50	1.65	1.59
1	C	13	DT	C4-O4	5.44	1.28	1.23
1	C	16	DT	C4-O4	5.41	1.28	1.23
1	C	18	DT	C4-O4	5.39	1.28	1.23
1	D	19	DG	O4'-C1'	5.37	1.48	1.42
1	D	6	DA	C8-N7	5.34	1.35	1.31
1	C	15	DT	O4'-C1'	5.30	1.48	1.42
1	C	2	DC	N3-C4	5.23	1.37	1.33
1	C	4	DG	P-OP2	5.21	1.57	1.49
1	D	11	DG	O3'-P	5.18	1.67	1.61
1	D	12	DA	C4'-O4'	-5.15	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	4	DG	O4'-C1'	5.10	1.48	1.42
1	D	9	DT	P-OP2	5.09	1.57	1.49

All (371) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	479	ARG	CD-NE-CZ	40.08	179.71	123.60
2	B	498	ARG	NE-CZ-NH2	-23.27	108.67	120.30
1	D	17	DC	O5'-P-OP2	22.34	137.51	110.70
1	D	17	DC	O4'-C4'-C3'	-21.38	93.17	106.00
1	D	19	DG	O4'-C4'-C3'	-20.73	93.56	106.00
1	C	16	DT	P-O3'-C3'	19.32	142.88	119.70
1	C	1	DC	P-O3'-C3'	19.01	142.51	119.70
1	C	13	DT	O4'-C1'-C2'	-17.68	91.76	105.90
1	D	5	DA	O5'-P-OP1	17.38	131.56	110.70
1	C	9	DT	O4'-C1'-N1	16.63	119.64	108.00
2	B	488	ARG	NE-CZ-NH1	-16.34	112.13	120.30
1	C	18	DT	O4'-C1'-C2'	-16.29	92.87	105.90
1	C	12	DA	O5'-P-OP1	16.02	129.92	110.70
1	C	6	DA	O4'-C4'-C3'	-15.93	96.44	106.00
1	C	2	DC	O4'-C4'-C3'	-15.72	96.57	106.00
1	D	18	DT	O4'-C1'-N1	15.64	118.95	108.00
1	D	10	DC	O4'-C4'-C3'	-15.22	96.86	106.00
1	D	19	DG	C1'-O4'-C4'	-15.21	94.89	110.10
1	D	7	DC	O4'-C1'-N1	15.15	118.61	108.00
1	D	11	DG	N3-C2-N2	14.94	130.36	119.90
1	D	2	DC	O4'-C1'-C2'	-14.89	93.99	105.90
1	C	1	DC	O4'-C4'-C3'	-14.74	97.16	106.00
1	D	15	DT	C2-N3-C4	-14.71	118.38	127.20
1	C	6	DA	O4'-C1'-N9	14.67	118.27	108.00
1	C	2	DC	O5'-P-OP1	14.59	128.20	110.70
2	B	498	ARG	CD-NE-CZ	-14.54	103.24	123.60
1	D	11	DG	N1-C2-N2	-14.53	103.12	116.20
1	C	5	DA	P-O3'-C3'	14.52	137.12	119.70
1	D	12	DA	O4'-C1'-C2'	-14.34	94.43	105.90
1	C	16	DT	O4'-C1'-N1	14.08	117.85	108.00
1	D	13	DT	C2-N3-C4	-13.90	118.86	127.20
1	C	19	DG	O4'-C4'-C3'	-13.73	97.76	106.00
1	D	13	DT	O4'-C1'-C2'	-13.26	95.29	105.90
2	B	496	ARG	NE-CZ-NH2	13.02	126.81	120.30
1	D	12	DA	P-O5'-C5'	-13.01	100.09	120.90
1	C	19	DG	OP1-P-OP2	-13.00	100.10	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	15	DT	O4'-C4'-C3'	-12.98	98.21	106.00
1	C	18	DT	P-O5'-C5'	-12.97	100.14	120.90
1	D	6	DA	O5'-P-OP1	12.39	125.56	110.70
1	C	14	DG	C6-N1-C2	-12.37	117.68	125.10
2	A	489	ARG	NE-CZ-NH1	12.32	126.46	120.30
1	C	15	DT	O4'-C1'-C2'	-12.24	96.11	105.90
1	D	16	DT	O4'-C1'-N1	12.22	116.55	108.00
1	D	15	DT	N1-C2-N3	12.05	121.83	114.60
1	C	19	DG	C4'-C3'-C2'	-11.82	92.46	103.10
1	C	13	DT	O4'-C4'-C3'	-11.76	98.94	106.00
2	A	497	TYR	CB-CG-CD1	11.74	128.05	121.00
1	C	14	DG	P-O3'-C3'	11.67	133.71	119.70
1	D	6	DA	N1-C2-N3	-11.65	123.48	129.30
1	C	6	DA	C4'-C3'-C2'	-11.63	92.63	103.10
1	D	9	DT	P-O5'-C5'	-11.51	102.48	120.90
1	D	18	DT	C2-N3-C4	-11.46	120.33	127.20
1	C	11	DG	O4'-C1'-N9	11.40	115.98	108.00
1	D	3	DA	OP1-P-OP2	11.32	136.58	119.60
1	C	12	DA	O4'-C4'-C3'	-11.23	99.26	106.00
1	D	11	DG	N1-C6-O6	-11.20	113.18	119.90
2	A	497	TYR	CB-CG-CD2	-11.16	114.30	121.00
2	A	488	ARG	NE-CZ-NH2	-11.00	114.80	120.30
1	C	12	DA	N1-C2-N3	-10.96	123.82	129.30
1	C	18	DT	N3-C4-O4	-10.91	113.36	119.90
1	C	14	DG	C5-C6-N1	10.84	116.92	111.50
1	D	1	DC	O4'-C1'-C2'	-10.84	97.23	105.90
2	A	481	ASP	CB-CG-OD2	10.81	128.03	118.30
1	D	6	DA	O4'-C4'-C3'	-10.78	99.53	106.00
1	C	14	DG	O4'-C1'-N9	10.74	115.52	108.00
1	D	17	DC	C1'-O4'-C4'	-10.59	99.51	110.10
1	D	4	DG	O4'-C1'-C2'	-10.55	97.46	105.90
2	B	489	ARG	NE-CZ-NH1	10.50	125.55	120.30
1	C	2	DC	C1'-O4'-C4'	-10.48	99.62	110.10
1	D	14	DG	O5'-P-OP2	10.42	123.21	110.70
1	C	13	DT	O5'-P-OP2	10.42	123.20	110.70
1	C	13	DT	C2-N3-C4	-10.40	120.96	127.20
1	C	3	DA	P-O5'-C5'	-10.29	104.44	120.90
1	D	16	DT	C2-N3-C4	-10.23	121.06	127.20
1	C	11	DG	P-O3'-C3'	10.22	131.97	119.70
1	C	9	DT	P-O3'-C3'	10.21	131.95	119.70
1	C	5	DA	C4'-C3'-C2'	-10.21	93.92	103.10
1	D	17	DC	O4'-C1'-C2'	-10.20	97.74	105.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	5	DA	O4'-C1'-C2'	-10.14	97.79	105.90
1	D	16	DT	N3-C4-O4	-10.13	113.82	119.90
1	C	16	DT	C2-N3-C4	-10.03	121.19	127.20
1	C	17	DC	P-O3'-C3'	-9.98	107.72	119.70
1	D	18	DT	N3-C4-C5	9.97	121.18	115.20
1	D	1	DC	P-O3'-C3'	9.94	131.63	119.70
1	D	9	DT	C2-N3-C4	-9.90	121.26	127.20
1	C	8	DA	O4'-C1'-C2'	-9.88	98.00	105.90
1	D	16	DT	C4'-C3'-C2'	-9.81	94.27	103.10
1	D	13	DT	N1-C2-N3	9.81	120.48	114.60
2	A	489	ARG	NE-CZ-NH2	-9.81	115.40	120.30
1	C	5	DA	P-O5'-C5'	-9.78	105.25	120.90
1	C	6	DA	P-O5'-C5'	-9.77	105.27	120.90
1	D	14	DG	O4'-C1'-N9	9.76	114.83	108.00
1	C	12	DA	C6-N1-C2	9.72	124.43	118.60
1	D	15	DT	N3-C4-C5	9.70	121.02	115.20
1	C	8	DA	P-O5'-C5'	-9.69	105.40	120.90
1	C	4	DG	O4'-C1'-N9	9.60	114.72	108.00
1	D	2	DC	O5'-P-OP2	9.60	122.21	110.70
2	B	481	ASP	CB-CG-OD1	9.58	126.92	118.30
1	D	18	DT	O4'-C4'-C3'	-9.55	100.27	106.00
1	D	4	DG	C5-C6-N1	9.51	116.26	111.50
2	A	498	ARG	CD-NE-CZ	-9.51	110.29	123.60
1	D	9	DT	O5'-P-OP2	-9.42	97.22	105.70
1	D	7	DC	C4'-C3'-C2'	-9.38	94.66	103.10
1	D	16	DT	C3'-C2'-C1'	-9.30	91.34	102.50
1	D	17	DC	N3-C4-C5	-9.28	118.19	121.90
2	B	485	ASP	CB-CA-C	9.24	128.88	110.40
1	C	12	DA	O4'-C1'-N9	9.21	114.45	108.00
1	C	1	DC	O4'-C1'-N1	-9.19	101.56	108.00
1	C	14	DG	N1-C2-N3	9.05	129.33	123.90
1	C	12	DA	P-O3'-C3'	8.97	130.46	119.70
1	C	18	DT	C2-N3-C4	-8.96	121.83	127.20
2	A	488	ARG	NE-CZ-NH1	8.93	124.77	120.30
2	A	446	GLU	OE1-CD-OE2	8.90	133.98	123.30
1	D	16	DT	C4-C5-C7	8.86	124.31	119.00
1	D	1	DC	O4'-C4'-C3'	-8.85	100.69	106.00
2	B	488	ARG	NH1-CZ-NH2	8.80	129.09	119.40
2	A	479	ARG	NE-CZ-NH1	8.78	124.69	120.30
1	C	16	DT	N3-C4-C5	8.72	120.43	115.20
1	C	2	DC	C4-C5-C6	-8.71	113.04	117.40
1	D	11	DG	P-O5'-C5'	-8.71	106.96	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	496	ARG	NE-CZ-NH1	-8.64	115.98	120.30
1	C	11	DG	C5-C6-O6	-8.63	123.42	128.60
1	C	12	DA	OP1-P-OP2	-8.60	106.70	119.60
1	D	11	DG	OP1-P-OP2	8.57	132.45	119.60
1	C	16	DT	O5'-P-OP1	8.56	120.98	110.70
1	C	16	DT	N1-C2-O2	-8.54	116.27	123.10
1	D	17	DC	OP1-P-OP2	-8.48	106.88	119.60
1	C	11	DG	O4'-C1'-C2'	-8.43	99.16	105.90
1	D	4	DG	C6-N1-C2	-8.40	120.06	125.10
1	C	18	DT	O5'-P-OP2	8.36	120.73	110.70
1	D	19	DG	O4'-C1'-N9	8.36	113.85	108.00
1	C	18	DT	N3-C4-C5	8.34	120.20	115.20
1	D	11	DG	C5-C6-O6	8.28	133.57	128.60
1	D	9	DT	N3-C4-C5	8.26	120.16	115.20
1	D	16	DT	N3-C4-C5	8.25	120.15	115.20
1	C	8	DA	C5-C6-N1	-8.24	113.58	117.70
1	C	12	DA	C5-C6-N1	-8.16	113.62	117.70
1	D	4	DG	O4'-C1'-N9	8.16	113.71	108.00
1	D	10	DC	C1'-O4'-C4'	-8.16	101.94	110.10
1	D	13	DT	N3-C2-O2	-8.13	117.42	122.30
1	C	15	DT	C6-C5-C7	-8.13	118.02	122.90
1	D	6	DA	C1'-O4'-C4'	-8.04	102.06	110.10
1	C	15	DT	C2-N3-C4	-8.04	122.38	127.20
1	C	14	DG	C4'-C3'-C2'	-8.04	95.87	103.10
1	C	3	DA	P-O3'-C3'	-8.00	110.10	119.70
1	D	5	DA	OP1-P-OP2	-7.95	107.68	119.60
1	D	17	DC	O5'-P-OP1	-7.94	98.56	105.70
1	D	13	DT	O4'-C4'-C3'	-7.91	101.25	106.00
1	C	2	DC	C5-C6-N1	7.89	124.95	121.00
2	A	438	ARG	NE-CZ-NH2	7.89	124.25	120.30
1	C	4	DG	O4'-C1'-C2'	-7.86	99.61	105.90
1	C	10	DC	O5'-P-OP2	7.81	120.07	110.70
1	C	4	DG	N1-C6-O6	-7.79	115.23	119.90
1	D	18	DT	C3'-C2'-C1'	-7.73	93.22	102.50
1	C	5	DA	N1-C2-N3	-7.71	125.44	129.30
1	D	7	DC	O4'-C4'-C3'	-7.70	101.38	106.00
1	D	15	DT	C6-N1-C2	-7.69	117.45	121.30
1	C	13	DT	N1-C2-N3	7.68	119.21	114.60
1	D	13	DT	N3-C4-C5	7.65	119.79	115.20
1	C	4	DG	N3-C2-N2	7.65	125.25	119.90
2	A	466	ARG	NE-CZ-NH1	7.63	124.12	120.30
1	D	16	DT	C6-C5-C7	-7.58	118.35	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	9	DT	C2-N3-C4	-7.58	122.65	127.20
1	D	11	DG	O4'-C1'-C2'	-7.52	99.88	105.90
1	C	15	DT	C4-C5-C7	7.50	123.50	119.00
1	C	5	DA	O4'-C4'-C3'	-7.48	101.51	104.50
1	C	18	DT	O4'-C4'-C3'	-7.48	101.51	104.50
1	C	19	DG	C5-C6-N1	7.46	115.23	111.50
2	A	466	ARG	O-C-N	-7.45	110.78	122.70
1	C	11	DG	C4'-C3'-C2'	-7.42	96.42	103.10
1	D	6	DA	OP1-P-OP2	-7.41	108.48	119.60
1	D	1	DC	C5-C6-N1	7.30	124.65	121.00
1	D	2	DC	O5'-P-OP1	7.26	119.41	110.70
1	D	14	DG	O4'-C1'-C2'	-7.25	100.10	105.90
2	A	473	ASN	O-C-N	7.24	134.28	122.70
2	A	466	ARG	NE-CZ-NH2	-7.23	116.68	120.30
1	C	17	DC	O4'-C1'-C2'	-7.23	100.11	105.90
1	C	9	DT	N1-C2-N3	7.22	118.93	114.60
2	B	505	MET	CG-SD-CE	7.21	111.73	100.20
1	C	3	DA	C8-N9-C4	-7.20	102.92	105.80
1	D	18	DT	OP1-P-O3'	7.20	121.03	105.20
1	C	18	DT	P-O3'-C3'	-7.19	111.08	119.70
1	D	7	DC	C3'-C2'-C1'	-7.12	93.95	102.50
2	A	488	ARG	NH1-CZ-NH2	-7.12	111.56	119.40
1	D	15	DT	N3-C2-O2	-7.12	118.03	122.30
2	B	501	LEU	O-C-N	-7.10	111.34	122.70
2	A	479	ARG	NH1-CZ-NH2	-7.08	111.61	119.40
1	D	6	DA	C6-N1-C2	7.06	122.84	118.60
1	D	13	DT	N3-C4-O4	-7.04	115.67	119.90
2	B	510	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	C	6	DA	C8-N9-C4	-7.04	102.98	105.80
1	C	19	DG	P-O5'-C5'	-7.03	109.66	120.90
1	C	11	DG	N1-C2-N3	7.02	128.11	123.90
1	D	8	DA	C5-C6-N1	-6.97	114.21	117.70
1	C	1	DC	C4'-C3'-C2'	-6.95	96.85	103.10
1	C	14	DG	O4'-C1'-C2'	-6.91	100.38	105.90
1	D	13	DT	O3'-P-O5'	-6.90	90.89	104.00
2	B	481	ASP	CA-C-O	-6.90	105.61	120.10
1	C	3	DA	O4'-C1'-C2'	-6.89	100.38	105.90
1	D	9	DT	OP1-P-OP2	-6.88	109.28	119.60
1	C	6	DA	O4'-C1'-C2'	-6.87	100.41	105.90
1	D	9	DT	N3-C4-O4	-6.83	115.80	119.90
1	C	3	DA	O4'-C1'-N9	6.82	112.77	108.00
1	C	15	DT	C1'-O4'-C4'	-6.75	103.35	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	10	DC	O3'-P-O5'	-6.74	91.19	104.00
1	C	2	DC	O5'-C5'-C4'	-6.72	94.19	111.00
1	D	18	DT	O5'-P-OP1	6.72	118.77	110.70
1	D	15	DT	P-O3'-C3'	6.72	127.76	119.70
1	D	18	DT	C5-C6-N1	-6.71	119.67	123.70
2	B	464	PHE	O-C-N	-6.71	111.97	122.70
1	D	10	DC	P-O3'-C3'	-6.70	111.66	119.70
1	C	3	DA	O4'-C4'-C3'	-6.67	101.83	104.50
1	D	14	DG	N3-C2-N2	-6.66	115.24	119.90
1	D	19	DG	C5-C6-O6	-6.66	124.61	128.60
1	D	15	DT	N3-C4-O4	-6.63	115.92	119.90
1	C	16	DT	N1-C2-N3	6.60	118.56	114.60
1	C	15	DT	P-O3'-C3'	6.59	127.61	119.70
1	D	7	DC	O4'-C1'-C2'	-6.59	100.63	105.90
1	D	16	DT	P-O3'-C3'	6.59	127.61	119.70
1	C	18	DT	OP1-P-OP2	6.58	129.48	119.60
1	C	17	DC	OP1-P-O3'	-6.58	90.73	105.20
1	C	13	DT	C5-C6-N1	-6.58	119.75	123.70
1	C	14	DG	N9-C4-C5	6.56	108.03	105.40
1	D	19	DG	C6-N1-C2	-6.52	121.19	125.10
2	B	510	ARG	CA-C-N	-6.51	102.87	117.20
2	A	498	ARG	NE-CZ-NH2	-6.49	117.05	120.30
1	C	11	DG	N1-C6-O6	6.41	123.74	119.90
2	B	494	ALA	N-CA-CB	6.40	119.07	110.10
1	D	2	DC	P-O3'-C3'	-6.40	112.02	119.70
1	C	11	DG	C6-N1-C2	-6.40	121.26	125.10
1	C	16	DT	OP1-P-OP2	-6.40	110.00	119.60
1	D	8	DA	P-O5'-C5'	-6.39	110.68	120.90
2	B	464	PHE	CA-C-O	6.39	133.51	120.10
1	D	17	DC	N1-C2-O2	6.35	122.71	118.90
1	C	18	DT	N3-C2-O2	-6.34	118.50	122.30
1	C	11	DG	OP2-P-O3'	-6.30	91.34	105.20
2	B	446	GLU	CG-CD-OE1	6.29	130.89	118.30
1	C	14	DG	N3-C4-C5	-6.27	125.47	128.60
1	C	8	DA	C6-N1-C2	6.27	122.36	118.60
1	C	15	DT	N1-C2-O2	-6.27	118.09	123.10
1	D	15	DT	OP1-P-OP2	-6.24	110.23	119.60
1	C	16	DT	C5-C4-O4	-6.23	120.54	124.90
1	D	13	DT	O4'-C1'-N1	-6.22	103.64	108.00
1	D	9	DT	N1-C2-N3	6.21	118.33	114.60
1	D	4	DG	N1-C2-N2	-6.20	110.62	116.20
2	B	498	ARG	NH1-CZ-NH2	6.20	126.22	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	15	DT	O4'-C1'-C2'	-6.18	100.95	105.90
1	D	16	DT	O4'-C4'-C3'	-6.16	102.04	104.50
1	D	14	DG	N9-C4-C5	6.15	107.86	105.40
1	C	11	DG	O5'-P-OP2	6.12	118.05	110.70
1	C	19	DG	C6-N1-C2	-6.12	121.43	125.10
2	B	511	LYS	CA-C-N	-6.12	103.73	117.20
1	C	17	DC	OP1-P-OP2	6.09	128.74	119.60
1	D	8	DA	O4'-C1'-N9	-6.07	103.75	108.00
2	B	474	TYR	CB-CG-CD2	-6.04	117.38	121.00
1	C	9	DT	C6-N1-C2	-6.03	118.29	121.30
1	D	4	DG	N1-C6-O6	-6.01	116.29	119.90
1	D	8	DA	C6-N1-C2	5.99	122.19	118.60
2	B	474	TYR	CA-CB-CG	5.99	124.78	113.40
2	B	510	ARG	CB-CA-C	5.97	122.34	110.40
1	D	10	DC	O4'-C1'-C2'	-5.96	101.14	105.90
1	D	14	DG	C6-N1-C2	-5.95	121.53	125.10
1	D	6	DA	C5-C6-N1	-5.95	114.73	117.70
1	D	9	DT	P-O3'-C3'	-5.94	112.57	119.70
1	C	3	DA	N9-C4-C5	5.91	108.16	105.80
1	C	3	DA	C1'-O4'-C4'	5.89	115.99	110.10
1	C	4	DG	N1-C2-N2	-5.89	110.90	116.20
1	D	11	DG	P-O3'-C3'	-5.88	112.64	119.70
1	D	14	DG	OP2-P-O3'	5.88	118.12	105.20
1	C	16	DT	P-O5'-C5'	-5.86	111.53	120.90
1	C	15	DT	N3-C4-C5	5.84	118.70	115.20
1	D	19	DG	C8-N9-C4	-5.84	104.06	106.40
2	B	446	GLU	OE1-CD-OE2	-5.83	116.30	123.30
2	B	511	LYS	C-N-CA	5.82	136.25	121.70
1	C	6	DA	P-O3'-C3'	-5.82	112.72	119.70
1	C	14	DG	C8-N9-C4	-5.80	104.08	106.40
1	C	11	DG	OP1-P-OP2	-5.79	110.91	119.60
1	D	19	DG	C4'-C3'-C2'	-5.79	97.89	103.10
1	D	2	DC	C5-C6-N1	5.78	123.89	121.00
1	D	15	DT	O4'-C1'-N1	5.76	112.03	108.00
1	C	7	DC	C5-C4-N4	5.75	124.23	120.20
1	C	15	DT	C5-C4-O4	-5.75	120.87	124.90
2	A	453	GLY	CA-C-O	-5.75	110.25	120.60
1	C	12	DA	N9-C1'-C2'	-5.74	101.69	112.60
1	D	14	DG	OP1-P-OP2	-5.73	111.00	119.60
2	A	451	HIS	C-N-CA	5.73	136.03	121.70
1	D	8	DA	OP1-P-O3'	5.73	117.80	105.20
1	C	19	DG	O5'-P-OP2	5.72	117.56	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	14	DG	N1-C6-O6	-5.70	116.48	119.90
2	B	434	MET	O-C-N	5.70	131.82	122.70
2	B	466	ARG	NE-CZ-NH1	-5.69	117.46	120.30
1	C	8	DA	C1'-O4'-C4'	-5.68	104.42	110.10
1	D	18	DT	O4'-C1'-C2'	-5.67	101.37	105.90
1	D	16	DT	O4'-C1'-C2'	-5.65	101.38	105.90
1	C	2	DC	C4'-C3'-C2'	-5.62	98.05	103.10
1	D	14	DG	P-O3'-C3'	5.61	126.43	119.70
1	C	7	DC	O5'-P-OP1	5.60	117.42	110.70
2	A	459	SER	CB-CA-C	-5.60	99.47	110.10
2	A	473	ASN	CB-CA-C	-5.56	99.28	110.40
1	C	16	DT	O5'-P-OP2	5.55	117.36	110.70
1	D	14	DG	C8-N9-C4	-5.55	104.18	106.40
2	A	499	LYS	C-N-CA	5.54	135.56	121.70
1	D	18	DT	N1-C2-N3	5.54	117.93	114.60
1	D	13	DT	P-O3'-C3'	-5.53	113.07	119.70
2	A	501	LEU	O-C-N	-5.53	113.86	122.70
1	C	19	DG	O4'-C1'-N9	5.51	111.86	108.00
1	D	19	DG	C5'-C4'-O4'	5.51	119.77	109.30
1	D	19	DG	C5-C6-N1	5.51	114.25	111.50
2	A	472	HIS	C-N-CA	5.51	135.47	121.70
2	A	438	ARG	CD-NE-CZ	5.50	131.30	123.60
2	B	445	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	D	17	DC	C2-N3-C4	5.46	122.63	119.90
1	D	8	DA	N1-C2-N3	-5.45	126.58	129.30
1	D	18	DT	C5-C4-O4	-5.43	121.10	124.90
1	D	11	DG	O4'-C1'-N9	5.43	111.80	108.00
2	B	438	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	C	17	DC	O3'-P-O5'	-5.39	93.75	104.00
1	C	16	DT	C4-C5-C7	5.38	122.23	119.00
2	B	477	ALA	CA-C-N	5.38	126.96	116.20
1	D	2	DC	OP1-P-O3'	-5.38	93.36	105.20
2	B	463	PHE	N-CA-CB	5.35	120.23	110.60
1	C	14	DG	N3-C2-N2	-5.34	116.17	119.90
1	C	2	DC	O4'-C1'-C2'	-5.33	101.63	105.90
1	D	2	DC	C4-C5-C6	-5.32	114.74	117.40
2	A	505	MET	CG-SD-CE	5.32	108.72	100.20
2	B	435	LYS	CB-CA-C	-5.32	99.76	110.40
1	C	6	DA	C5'-C4'-C3'	-5.31	104.54	114.10
1	C	7	DC	OP1-P-O3'	5.28	116.82	105.20
1	D	7	DC	OP1-P-OP2	-5.28	111.68	119.60
1	C	10	DC	C5-C6-N1	5.27	123.64	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	462	VAL	CB-CA-C	-5.27	101.39	111.40
2	A	457	CYS	CA-CB-SG	5.26	123.47	114.00
1	C	9	DT	C6-N1-C1'	5.26	128.29	120.40
2	B	466	ARG	CG-CD-NE	-5.25	100.77	111.80
2	A	468	VAL	CA-CB-CG1	5.25	118.77	110.90
1	C	13	DT	N3-C4-C5	5.24	118.35	115.20
1	D	19	DG	OP1-P-OP2	-5.24	111.74	119.60
2	B	489	ARG	CD-NE-CZ	5.24	130.93	123.60
2	A	447	ALA	N-CA-CB	-5.22	102.78	110.10
2	B	444	SER	O-C-N	-5.21	114.36	122.70
1	D	2	DC	OP1-P-OP2	-5.18	111.83	119.60
1	D	16	DT	N1-C2-N3	5.18	117.71	114.60
2	B	444	SER	N-CA-CB	-5.17	102.74	110.50
1	C	7	DC	O4'-C1'-N1	5.17	111.62	108.00
2	A	474	TYR	N-CA-CB	-5.17	101.30	110.60
1	C	8	DA	O5'-P-OP1	-5.16	101.05	105.70
1	D	11	DG	O5'-C5'-C4'	-5.16	98.09	111.00
2	B	480	ASN	CB-CG-OD1	5.16	131.92	121.60
2	B	510	ARG	N-CA-CB	5.15	119.87	110.60
2	A	458	GLY	C-N-CA	5.14	134.54	121.70
1	C	9	DT	O5'-C5'-C4'	-5.13	98.17	111.00
1	C	10	DC	P-O3'-C3'	-5.13	113.54	119.70
1	C	13	DT	P-O3'-C3'	-5.13	113.55	119.70
1	D	19	DG	N7-C8-N9	5.11	115.65	113.10
1	C	1	DC	C1'-O4'-C4'	-5.10	105.00	110.10
2	B	482	CYS	O-C-N	5.10	130.86	122.70
1	C	5	DA	C5-C6-N1	-5.10	115.15	117.70
2	B	436	PRO	N-CA-C	-5.08	98.88	112.10
1	D	1	DC	N1-C2-O2	5.08	121.95	118.90
1	D	8	DA	OP2-P-O3'	5.08	116.36	105.20
1	C	8	DA	C8-N9-C4	-5.07	103.77	105.80
1	D	6	DA	OP2-P-O3'	5.07	116.35	105.20
2	B	469	GLU	OE1-CD-OE2	5.07	129.38	123.30
2	B	486	LYS	O-C-N	-5.07	114.59	122.70
2	B	503	ALA	O-C-N	-5.06	114.60	123.20
2	A	467	ALA	C-N-CA	5.05	134.33	121.70
1	D	5	DA	O4'-C1'-N9	-5.05	104.47	108.00
2	B	466	ARG	CA-CB-CG	5.05	124.50	113.40
1	C	10	DC	N3-C4-C5	-5.01	119.90	121.90
1	D	2	DC	C3'-C2'-C1'	-5.01	96.49	102.50
1	D	16	DT	OP1-P-OP2	-5.01	112.09	119.60

There are no chirality outliers.

All (27) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	437	ALA	Mainchain
2	A	450	CYS	Mainchain
2	A	466	ARG	Mainchain
2	A	482	CYS	Mainchain
2	A	488	ARG	Sidechain
2	A	496	ARG	Sidechain,Mainchain
2	A	498	ARG	Sidechain
2	B	441	LEU	Mainchain
2	B	451	HIS	Mainchain
2	B	452	TYR	Sidechain
2	B	463	PHE	Mainchain
2	B	466	ARG	Sidechain
2	B	468	VAL	Mainchain
2	B	471	GLN	Mainchain
2	B	485	ASP	Mainchain
2	B	491	ASN	Mainchain
2	B	497	TYR	Sidechain
2	B	498	ARG	Sidechain
2	B	501	LEU	Mainchain
2	B	502	GLN	Sidechain
1	C	19	DG	Sidechain
1	C	2	DC	Sidechain
1	D	12	DA	Sidechain
1	D	17	DC	Sidechain
1	D	19	DG	Sidechain
1	D	8	DA	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	C	385	0	216	20	1
1	D	385	0	216	23	0
2	A	619	0	623	54	0
2	B	619	0	623	42	1
3	A	2	0	0	0	0
3	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	32	0	0	3	0
4	B	41	0	0	7	0
4	C	23	0	0	3	0
4	D	13	0	0	6	0
All	All	2121	0	1678	126	2

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 38.

All (126) 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:484:ILE:O	2:B:485:ASP:HB3	1.42	1.16
1:D:6:DA:H2"	1:D:7:DC:H5'	1.28	1.12
1:D:8:DA:H2"	1:D:9:DT:O5'	1.62	1.00
1:D:16:DT:O4	4:D:32:HOH:O	1.78	0.99
2:B:443:CYS:O	2:B:444:SER:HB2	1.63	0.95
1:D:16:DT:H73	4:D:32:HOH:O	1.67	0.94
2:B:471:GLN:HA	4:B:13:HOH:O	1.67	0.94
2:A:486:LYS:HG2	2:A:486:LYS:O	1.69	0.90
2:A:475:LEU:HD12	2:B:488:ARG:NH2	1.87	0.90
2:B:484:ILE:O	2:B:485:ASP:CB	2.20	0.90
2:A:511:LYS:O	2:A:512:THR:HB	1.75	0.87
1:D:6:DA:C2'	1:D:7:DC:H5'	2.05	0.86
1:D:16:DT:O5'	1:D:16:DT:H2'	1.76	0.83
2:A:456:THR:CG2	2:A:457:CYS:N	2.41	0.83
1:C:7:DC:H2"	1:C:8:DA:O5'	1.79	0.82
1:C:5:DA:OP2	4:C:31:HOH:O	1.98	0.81
1:D:18:DT:O5'	1:D:18:DT:H2'	1.81	0.80
1:C:5:DA:N6	1:D:16:DT:O4	2.15	0.80
1:D:16:DT:C7	4:D:32:HOH:O	2.29	0.78
1:C:18:DT:H2"	1:C:19:DG:H5"	1.67	0.76
2:B:484:ILE:HD12	4:B:55:HOH:O	1.84	0.76
1:D:10:DC:H2'	1:D:11:DG:C8	2.21	0.76
2:A:456:THR:CG2	2:A:457:CYS:H	2.02	0.72
2:A:456:THR:HG22	2:A:457:CYS:N	2.03	0.72
2:A:456:THR:HG23	2:A:457:CYS:H	1.53	0.72
2:A:511:LYS:O	2:A:512:THR:CB	2.38	0.72
2:A:465:LYS:HZ2	2:A:469:GLU:CD	1.94	0.70
1:C:14:DG:O5'	1:C:14:DG:H2'	1.91	0.69
1:C:10:DC:H2"	1:C:11:DG:H5'	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:437:ALA:O	2:A:438:ARG:HB2	1.94	0.67
2:A:446:GLU:O	4:A:105:HOH:O	2.11	0.67
2:A:452:TYR:HB3	2:A:506:ASN:O	1.94	0.67
2:A:439:PRO:O	2:A:439:PRO:HG2	1.96	0.66
2:A:475:LEU:CD1	2:B:488:ARG:NH2	2.58	0.66
2:B:437:ALA:HB1	4:B:3:HOH:O	1.95	0.66
2:B:501:LEU:O	2:B:503:ALA:N	2.29	0.66
1:D:11:DG:O5'	1:D:11:DG:H2'	1.96	0.65
2:B:437:ALA:CB	4:B:3:HOH:O	2.44	0.64
2:B:435:LYS:HD2	2:B:446:GLU:OE2	1.99	0.63
1:D:9:DT:H2"	1:D:10:DC:OP2	1.97	0.63
2:A:498:ARG:HH21	2:A:498:ARG:HB3	1.64	0.61
1:C:18:DT:H2"	1:C:19:DG:C5'	2.31	0.59
2:B:481:ASP:CG	2:B:481:ASP:O	2.41	0.59
1:D:16:DT:O5'	1:D:16:DT:C2'	2.49	0.59
1:D:14:DG:O6	2:A:466:ARG:NH1	2.29	0.59
2:B:448:SER:OG	2:B:451:HIS:HE1	1.86	0.59
2:A:437:ALA:O	2:A:438:ARG:CB	2.51	0.58
2:B:462:VAL:O	2:B:466:ARG:HB2	2.04	0.58
2:B:483:ILE:HD13	2:B:483:ILE:N	2.20	0.57
1:C:10:DC:H2"	1:C:11:DG:C5'	2.34	0.57
2:B:484:ILE:HB	4:B:55:HOH:O	2.04	0.57
2:B:443:CYS:O	2:B:444:SER:CB	2.38	0.57
1:C:2:DC:H1'	2:A:511:LYS:HD3	1.86	0.57
2:A:497:TYR:O	2:A:500:CYS:HB2	2.05	0.57
2:A:488:ARG:HD2	2:B:477:ALA:HA	1.86	0.56
1:C:2:DC:H2'	1:C:3:DA:C8	2.40	0.56
2:A:488:ARG:NH2	2:B:475:LEU:HD13	2.20	0.56
1:C:7:DC:C2'	1:C:8:DA:O5'	2.51	0.56
2:A:465:LYS:O	2:A:469:GLU:HG3	2.06	0.56
2:A:468:VAL:HG23	2:A:469:GLU:N	2.19	0.56
4:D:26:HOH:O	2:B:511:LYS:HE3	2.06	0.55
2:B:509:ALA:C	2:B:511:LYS:N	2.52	0.55
2:A:439:PRO:O	2:A:439:PRO:CG	2.55	0.55
1:D:16:DT:C4	4:D:32:HOH:O	2.48	0.54
2:A:496:ARG:O	2:A:497:TYR:C	2.46	0.53
2:A:447:ALA:HB1	2:A:455:LEU:CD1	2.38	0.53
4:D:24:HOH:O	2:A:451:HIS:HE1	1.90	0.53
2:A:465:LYS:NZ	2:A:469:GLU:CD	2.62	0.52
1:D:9:DT:C2'	1:D:10:DC:OP2	2.53	0.52
2:B:472:HIS:N	4:B:13:HOH:O	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:11:DG:O5'	1:D:11:DG:C2'	2.58	0.52
1:C:2:DC:P	4:C:28:HOH:O	2.68	0.51
1:C:2:DC:H2"	2:A:511:LYS:HE3	1.92	0.51
1:D:8:DA:C2'	1:D:9:DT:O5'	2.47	0.51
2:A:468:VAL:HG23	2:A:469:GLU:H	1.75	0.51
2:B:468:VAL:HG23	2:B:469:GLU:N	2.26	0.50
2:B:501:LEU:O	2:B:502:GLN:C	2.48	0.50
2:A:475:LEU:HD12	2:B:488:ARG:HH21	1.75	0.49
2:A:456:THR:HG22	2:A:457:CYS:O	2.12	0.49
2:A:498:ARG:NH2	4:A:72:HOH:O	2.28	0.49
2:B:511:LYS:NZ	2:B:511:LYS:HB2	2.27	0.49
1:D:18:DT:O5'	1:D:18:DT:C2'	2.52	0.49
2:A:485:ASP:O	2:A:489:ARG:HB3	2.12	0.48
1:C:14:DG:O5'	1:C:14:DG:C2'	2.49	0.48
1:C:18:DT:C2'	1:C:19:DG:H5"	2.42	0.48
2:A:438:ARG:N	2:A:439:PRO:CD	2.77	0.48
2:A:488:ARG:HH22	2:B:475:LEU:HD13	1.79	0.48
2:A:501:LEU:O	2:A:502:GLN:C	2.52	0.47
2:B:479:ARG:NH1	4:B:76:HOH:O	2.48	0.47
2:A:447:ALA:CB	2:A:455:LEU:HD11	2.45	0.46
2:A:462:VAL:O	2:A:466:ARG:HB2	2.15	0.46
2:A:498:ARG:NH1	4:A:72:HOH:O	2.43	0.46
2:B:487:ILE:H	2:B:487:ILE:HG12	1.18	0.46
2:A:447:ALA:HB1	2:A:455:LEU:HD11	1.97	0.46
2:A:447:ALA:HA	2:A:456:THR:O	2.16	0.46
1:D:13:DT:H2"	1:D:14:DG:O5'	2.16	0.45
2:A:475:LEU:HB3	2:B:488:ARG:HD3	1.98	0.45
2:B:483:ILE:HG22	2:B:484:ILE:H	1.82	0.45
2:A:485:ASP:O	2:A:486:LYS:C	2.53	0.44
2:B:484:ILE:HD11	2:B:496:ARG:HG3	2.00	0.44
2:A:481:ASP:OD1	2:A:481:ASP:C	2.56	0.44
2:B:501:LEU:HA	2:B:501:LEU:HD12	1.58	0.44
1:C:11:DG:H1	1:D:10:DC:N4	2.15	0.43
1:C:6:DA:H2'	1:C:6:DA:H5'	1.22	0.43
2:B:483:ILE:HG22	2:B:484:ILE:N	2.33	0.43
2:B:464:PHE:O	2:B:465:LYS:C	2.56	0.43
2:B:465:LYS:O	2:B:469:GLU:HG3	2.18	0.43
2:B:498:ARG:HH21	2:B:498:ARG:HD2	1.10	0.43
2:A:459:SER:HB2	2:A:496:ARG:NH1	2.33	0.43
2:A:465:LYS:NZ	2:A:469:GLU:OE2	2.47	0.42
2:B:488:ARG:HH21	2:B:488:ARG:HD3	1.65	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:510:ARG:HH21	2:A:510:ARG:HD2	1.68	0.42
2:A:438:ARG:H	2:A:455:LEU:HD21	1.85	0.41
1:C:15:DT:H2"	1:C:16:DT:H5'	2.01	0.41
2:A:507:LEU:HD12	2:A:507:LEU:HA	1.87	0.41
2:B:447:ALA:CB	2:B:455:LEU:HD23	2.51	0.41
2:B:507:LEU:HD23	2:B:507:LEU:HA	1.85	0.41
1:C:12:DA:N3	4:C:34:HOH:O	2.37	0.41
1:D:17:DC:H2'	1:D:18:DT:C6	2.56	0.41
1:C:19:DG:H5'	1:C:19:DG:H2'	1.20	0.40
2:A:448:SER:N	2:A:456:THR:O	2.49	0.40
2:B:511:LYS:HB3	2:B:512:THR:H	1.21	0.40
1:D:13:DT:H4'	2:A:490:LYS:HE3	2.03	0.40
2:A:438:ARG:HA	2:A:438:ARG:HD3	1.84	0.40
2:A:472:HIS:HB3	2:A:473:ASN:H	1.68	0.40
2:B:465:LYS:NZ	2:B:469:GLU:CD	2.75	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:DC:N3	1:C:19:DG:N7[2_455]	1.98	0.22
2:B:488:ARG:NH1	2:B:498:ARG:NE[4_555]	2.02	0.18

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	78/92 (85%)	63 (81%)	10 (13%)	5 (6%)	1	1
2	B	78/92 (85%)	66 (85%)	9 (12%)	3 (4%)	3	4
All	All	156/184 (85%)	129 (83%)	19 (12%)	8 (5%)	2	2

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	438	ARG
2	B	512	THR
2	A	439	PRO
2	B	501	LEU
2	A	497	TYR
2	A	512	THR
2	B	485	ASP
2	A	498	ARG

5.3.2 Protein sidechains (i)

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	67/75 (89%)	53 (79%)	14 (21%)	1 2
2	B	67/75 (89%)	50 (75%)	17 (25%)	0 1
All	All	134/150 (89%)	103 (77%)	31 (23%)	1 1

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	434	MET
2	A	438	ARG
2	A	439	PRO
2	A	454	VAL
2	A	459	SER
2	A	462	VAL
2	A	471	GLN
2	A	473	ASN
2	A	475	LEU
2	A	479	ARG
2	A	486	LYS
2	A	498	ARG
2	A	510	ARG
2	A	513	LYS
2	B	434	MET

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Mol	Chain	Res	Type
2	B	435	LYS
2	B	438	ARG
2	B	439	PRO
2	B	450	CYS
2	B	455	LEU
2	B	474	TYR
2	B	479	ARG
2	B	487	ILE
2	B	488	ARG
2	B	490	LYS
2	B	491	ASN
2	B	493	PRO
2	B	499	LYS
2	B	501	LEU
2	B	510	ARG
2	B	511	LYS

Sometimes 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	480	ASN
2	B	491	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 monosaccharides in this entry.

5.6 Ligand geometry

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

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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.