



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 03:50 PM GMT

PDB ID : 3D1N  
Title : Structure of human Brn-5 transcription factor in complex with corticotrophin  
-releasing hormone gene promoter  
Authors : Pereira, J.H.; Ha, S.C.; Kim, S.-H.  
Deposited on : 2008-05-06  
Resolution : 2.51 Å (reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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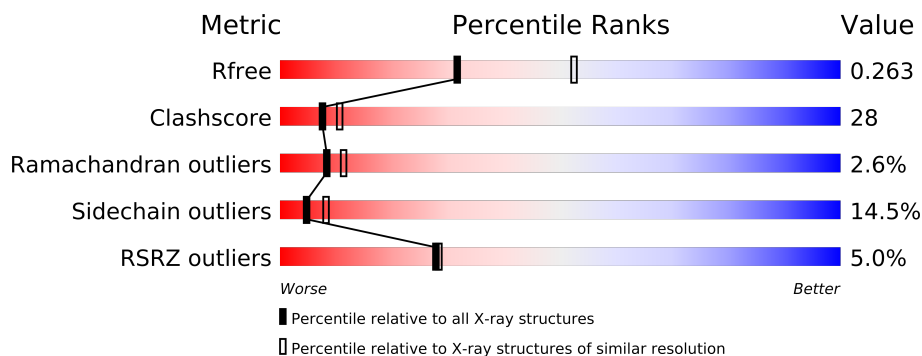
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.51 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	14	
1	C	14	
1	E	14	
1	G	14	
2	B	14	
2	D	14	
2	F	14	
2	H	14	
3	I	151	
3	J	151	
3	K	151	
3	L	151	
3	M	151	
3	N	151	

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Mol	Chain	Length	Quality of chain
3	O	151	
3	P	151	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10089 atoms, of which 0 are hydrogen and 0 are deuterium.

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(\*DAP\*DGP\*DCP\*DAP\*DTP\*DAP\*DAP\*DTP\*DAP\*DAP\*DTP\*DAP\*DA)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	14	Total	C	N	O	P	0	0	0
			287	139	59	76	13			
1	C	14	Total	C	N	O	P	0	0	0
			287	139	59	76	13			
1	E	14	Total	C	N	O	P	0	0	0
			287	139	59	76	13			
1	G	14	Total	C	N	O	P	0	0	0
			287	139	59	76	13			

- Molecule 2 is a DNA chain called 5'-D(\*DTP\*DTP\*DAP\*DTP\*DTP\*DAP\*DTP\*DTP\*DTP\*DAP\*DTP\*DGP\*DCP\*DT)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	14	Total	C	N	O	P	0	0	0
			281	139	41	88	13			
2	D	14	Total	C	N	O	P	0	0	0
			281	139	41	88	13			
2	F	14	Total	C	N	O	P	0	0	0
			281	139	41	88	13			
2	H	14	Total	C	N	O	P	0	0	0
			281	139	41	88	13			

- Molecule 3 is a protein called POU domain, class 6, transcription factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	150	Total	C	N	O	Se	0	0	0
			1192	746	216	226	4			
3	J	86	Total	C	N	O	Se	0	0	0
			666	420	114	129	3			
3	K	150	Total	C	N	O	Se	0	0	0
			1100	689	194	213	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	145	Total	C	N	O	Se	0	0	0
			1130	708	203	215	4			
3	M	150	Total	C	N	O	Se	0	0	0
			1188	742	215	227	4			
3	N	85	Total	C	N	O	Se	0	0	0
			658	414	113	128	3			
3	O	150	Total	C	N	O	Se	0	0	0
			1166	730	209	223	4			
3	P	82	Total	C	N	O	Se	0	0	0
			620	390	108	119	3			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	144	MSE	LEU	ENGINEERED	UNP Q14863
I	172	MSE	LEU	ENGINEERED	UNP Q14863
I	186	SER	CYS	ENGINEERED	UNP Q14863
I	267	MSE	ILE	ENGINEERED	UNP Q14863
I	283	SER	CYS	ENGINEERED	UNP Q14863
J	144	MSE	LEU	ENGINEERED	UNP Q14863
J	172	MSE	LEU	ENGINEERED	UNP Q14863
J	186	SER	CYS	ENGINEERED	UNP Q14863
J	267	MSE	ILE	ENGINEERED	UNP Q14863
J	283	SER	CYS	ENGINEERED	UNP Q14863
K	144	MSE	LEU	ENGINEERED	UNP Q14863
K	172	MSE	LEU	ENGINEERED	UNP Q14863
K	186	SER	CYS	ENGINEERED	UNP Q14863
K	267	MSE	ILE	ENGINEERED	UNP Q14863
K	283	SER	CYS	ENGINEERED	UNP Q14863
L	144	MSE	LEU	ENGINEERED	UNP Q14863
L	172	MSE	LEU	ENGINEERED	UNP Q14863
L	186	SER	CYS	ENGINEERED	UNP Q14863
L	267	MSE	ILE	ENGINEERED	UNP Q14863
L	283	SER	CYS	ENGINEERED	UNP Q14863
M	144	MSE	LEU	ENGINEERED	UNP Q14863
M	172	MSE	LEU	ENGINEERED	UNP Q14863
M	186	SER	CYS	ENGINEERED	UNP Q14863
M	267	MSE	ILE	ENGINEERED	UNP Q14863
M	283	SER	CYS	ENGINEERED	UNP Q14863
N	144	MSE	LEU	ENGINEERED	UNP Q14863
N	172	MSE	LEU	ENGINEERED	UNP Q14863
N	186	SER	CYS	ENGINEERED	UNP Q14863
N	267	MSE	ILE	ENGINEERED	UNP Q14863

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Chain	Residue	Modelled	Actual	Comment	Reference
N	283	SER	CYS	ENGINEERED	UNP Q14863
O	144	MSE	LEU	ENGINEERED	UNP Q14863
O	172	MSE	LEU	ENGINEERED	UNP Q14863
O	186	SER	CYS	ENGINEERED	UNP Q14863
O	267	MSE	ILE	ENGINEERED	UNP Q14863
O	283	SER	CYS	ENGINEERED	UNP Q14863
P	144	MSE	LEU	ENGINEERED	UNP Q14863
P	172	MSE	LEU	ENGINEERED	UNP Q14863
P	186	SER	CYS	ENGINEERED	UNP Q14863
P	267	MSE	ILE	ENGINEERED	UNP Q14863
P	283	SER	CYS	ENGINEERED	UNP Q14863

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	9	Total O 9 9	0	0
4	B	10	Total O 10 10	0	0
4	C	5	Total O 5 5	0	0
4	D	1	Total O 1 1	0	0
4	E	9	Total O 9 9	0	0
4	F	10	Total O 10 10	0	0
4	G	4	Total O 4 4	0	0
4	H	5	Total O 5 5	0	0
4	I	8	Total O 8 8	0	0
4	J	6	Total O 6 6	0	0
4	L	1	Total O 1 1	0	0
4	M	10	Total O 10 10	0	0
4	N	6	Total O 6 6	0	0
4	O	10	Total O 10 10	0	0

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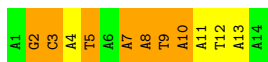
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	P	3	Total	O	0	0
			3	3		

### 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 errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 5'-D(\*DAP\*DGP\*DCP\*DAP\*DTP\*DAP\*DAP\*DAP\*DTP\*DAP\*DAP\*DTP\*DAP\*DA)-3'

Chain A: 



- Molecule 1: 5'-D(\*DAP\*DGP\*DCP\*DAP\*DTP\*DAP\*DAP\*DAP\*DTP\*DAP\*DAP\*DTP\*DAP\*DA)-3'

Chain C: 



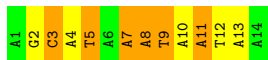
- Molecule 1: 5'-D(\*DAP\*DGP\*DCP\*DAP\*DTP\*DAP\*DAP\*DAP\*DTP\*DAP\*DAP\*DTP\*DAP\*DA)-3'

Chain E: 



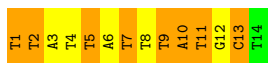
- Molecule 1: 5'-D(\*DAP\*DGP\*DCP\*DAP\*DTP\*DAP\*DAP\*DAP\*DTP\*DAP\*DAP\*DTP\*DAP\*DA)-3'

Chain G: 



- Molecule 2: 5'-D(\*DTP\*DTP\*DAP\*DTP\*DTP\*DAP\*DTP\*DTP\*DTP\*DAP\*DTP\*DGP\*DCP\*DT)-3'

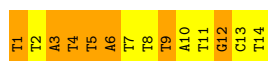
Chain B: 



- Molecule 2: 5'-D(\*DTP\*DTP\*DAP\*DTP\*DTP\*DAP\*DTP\*DTP\*DTP\*DAP\*DTP\*DGP\*DCP\*DT)-3'

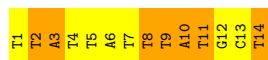
Chain D: 





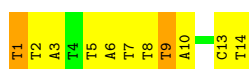
- Molecule 2: 5'-D(\*DTP\*DTP\*DAP\*DTP\*DTP\*DAP\*DTP\*DTP\*DTP\*DAP\*DTP\*DGP\*D CP\*DT)-3'

Chain F:



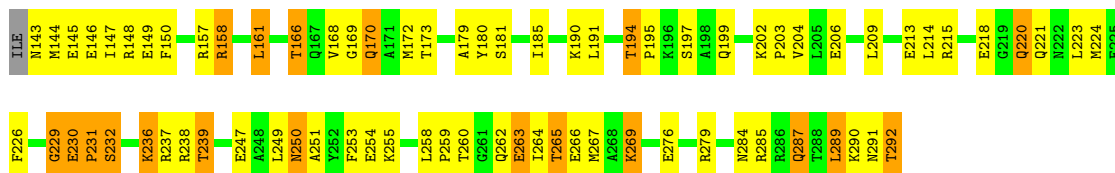
- Molecule 2: 5'-D(\*DTP\*DTP\*DAP\*DTP\*DTP\*DAP\*DTP\*DTP\*DTP\*DAP\*DTP\*DGP\*D CP\*DT)-3'

Chain H:



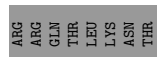
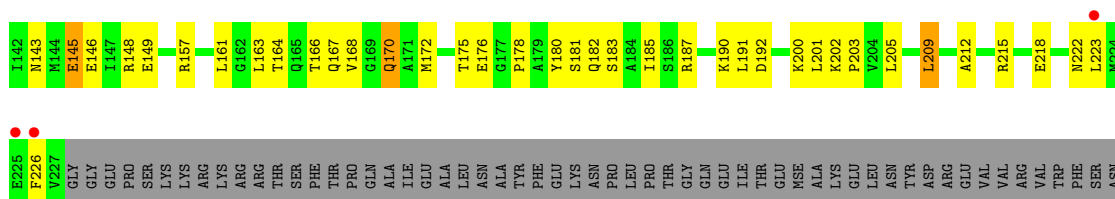
- Molecule 3: POU domain, class 6, transcription factor 1

Chain I:



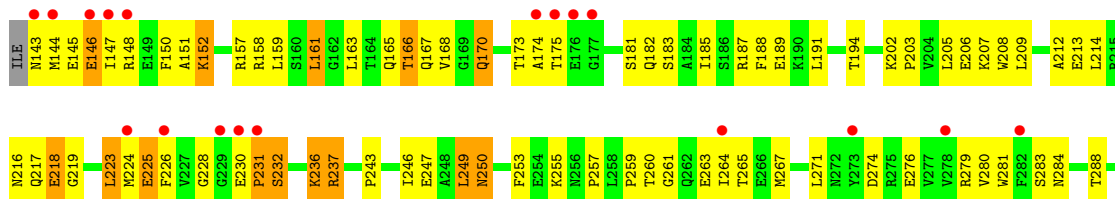
- Molecule 3: POU domain, class 6, transcription factor 1

Chain J:



- Molecule 3: POU domain, class 6, transcription factor 1

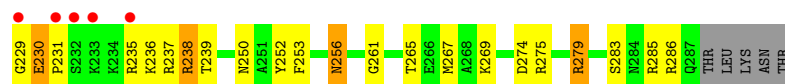
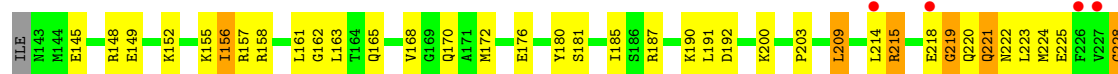
Chain K:





- Molecule 3: POU domain, class 6, transcription factor 1

Chain L:



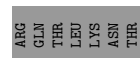
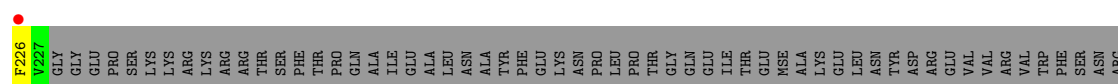
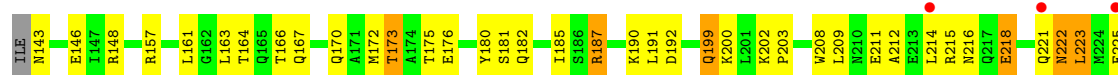
- Molecule 3: POU domain, class 6, transcription factor 1

Chain M:



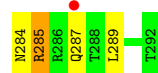
- Molecule 3: POU domain, class 6, transcription factor 1

Chain N:



- Molecule 3: POU domain, class 6, transcription factor 1

Chain O:



- Molecule 3: POU domain, class 6, transcription factor 1

Chain P:

THR	PRO	GLN	ALA	ILE	GLU	ALA	LEU	ASN	ALA	TYR	PHE	GLU	GLY	LYS	ASN	PRO	LEU	PRO	THR	GLY	GLN	GLU	ILE	THR	GLU	NSE	ALA	LYS	GLU	LEU	ASN	TYR	ASP	ARG	GLU	VAL	ARG	VAL	TRP	PHE	SER	ASN	ARG	ARG	GLN	THR	LEU	LYS	ASN	THR
M143	M144	I147	K155	I156	R157	R158	L161	G162	L163	T164	Q165	T166	Q167	V168	M172	T173	A174	T175	E176	G177	P178	Q182	K190	K202	P203	L209	L214	R215	N216	L223	M224	GLU	PHE	VAL	GLY	GLY	GLY	PRO	SER	LYS	LYS	ARG	LYS	ARG	ARG	THR	SER	PHE		

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	100.30Å 112.06Å 181.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.91 – 2.51 48.91 – 2.51	Depositor EDS
% Data completeness (in resolution range)	91.0 (48.91-2.51) 74.7 (48.91-2.51)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	65.06 (at 2.51Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.212 , 0.270 0.207 , 0.263	Depositor DCC
$R_{free}$ test set	2670 reflections (5.10%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.8	Xtriage
Anisotropy	0.886	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 49.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	5 of 52734 reflections (0.009%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10089	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.17% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.80	0/324	1.84	11/498 (2.2%)
1	C	0.79	0/324	1.89	13/498 (2.6%)
1	E	0.95	0/324	1.93	13/498 (2.6%)
1	G	0.87	0/324	1.89	12/498 (2.4%)
2	B	0.83	0/312	1.95	13/480 (2.7%)
2	D	0.85	0/312	2.17	15/480 (3.1%)
2	F	0.85	0/312	2.19	21/480 (4.4%)
2	H	0.96	0/312	2.03	10/480 (2.1%)
3	I	0.42	0/1208	0.59	0/1622
3	J	0.41	0/672	0.57	0/900
3	K	0.29	0/1114	0.52	0/1507
3	L	0.36	0/1146	0.55	0/1540
3	M	0.42	0/1204	0.65	0/1620
3	N	0.41	0/664	0.60	0/889
3	O	0.36	0/1182	0.55	0/1593
3	P	0.38	0/625	0.55	0/836
All	All	0.54	0/10359	1.15	108/14419 (0.7%)

There are no bond length outliers.

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	5	DT	O4'-C1'-N1	-13.05	98.87	108.00
2	D	9	DT	O4'-C1'-N1	13.04	117.13	108.00
2	D	12	DG	O4'-C1'-N9	-11.20	100.16	108.00
2	D	5	DT	O4'-C1'-N1	-10.91	100.36	108.00
1	A	5	DT	O4'-C1'-N1	10.16	115.11	108.00
1	C	2	DG	O4'-C1'-N9	10.13	115.09	108.00
2	H	13	DC	O4'-C4'-C3'	-9.95	100.03	106.00
1	C	5	DT	O4'-C1'-N1	9.80	114.86	108.00
1	E	5	DT	O4'-C1'-N1	9.60	114.72	108.00
1	A	7	DA	O4'-C1'-N9	-9.49	101.36	108.00
1	A	8	DA	O4'-C1'-N9	-9.09	101.64	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	2	DG	C4'-C3'-C2'	-9.07	94.94	103.10
1	G	13	DA	O4'-C1'-C2'	-8.84	98.83	105.90
1	C	7	DA	O4'-C1'-N9	-8.65	101.94	108.00
2	F	9	DT	O4'-C1'-N1	-8.54	102.02	108.00
1	C	1	DA	O4'-C1'-N9	8.47	113.93	108.00
1	C	3	DC	O4'-C1'-N1	-8.04	102.37	108.00
1	E	3	DC	O4'-C1'-N1	-8.01	102.39	108.00
2	D	7	DT	O4'-C1'-N1	-7.73	102.59	108.00
2	H	3	DA	O4'-C1'-N9	-7.72	102.60	108.00
2	F	12	DG	O4'-C1'-N9	-7.54	102.73	108.00
2	D	8	DT	O4'-C1'-N1	-7.50	102.75	108.00
1	C	1	DA	C1'-O4'-C4'	-7.39	102.70	110.10
2	F	14	DT	C6-C5-C7	-7.39	118.47	122.90
2	F	2	DT	C5-C4-O4	-7.34	119.76	124.90
1	G	9	DT	N3-C4-O4	7.26	124.25	119.90
1	E	7	DA	O4'-C1'-N9	-7.18	102.97	108.00
1	C	8	DA	O4'-C1'-N9	-7.16	102.99	108.00
2	D	1	DT	N3-C4-O4	7.13	124.18	119.90
1	G	9	DT	C5-C4-O4	-6.98	120.02	124.90
2	H	8	DT	O4'-C1'-N1	-6.98	103.12	108.00
2	F	13	DC	C1'-O4'-C4'	-6.89	103.21	110.10
2	D	4	DT	O4'-C1'-N1	-6.84	103.21	108.00
1	G	11	DA	O4'-C1'-N9	-6.81	103.23	108.00
2	F	13	DC	O4'-C4'-C3'	-6.79	101.78	104.50
1	C	12	DT	O4'-C1'-C2'	-6.68	100.56	105.90
2	B	5	DT	N3-C4-O4	6.54	123.83	119.90
2	H	13	DC	P-O3'-C3'	6.47	127.47	119.70
2	B	2	DT	O4'-C1'-N1	-6.44	103.49	108.00
2	H	9	DT	N3-C2-O2	-6.43	118.44	122.30
2	F	3	DA	O4'-C1'-N9	-6.41	103.51	108.00
1	G	8	DA	O4'-C1'-N9	-6.40	103.52	108.00
2	H	1	DT	O4'-C1'-N1	-6.31	103.58	108.00
2	F	2	DT	N3-C4-O4	6.27	123.66	119.90
2	D	12	DG	O4'-C1'-C2'	-6.22	100.93	105.90
2	D	8	DT	P-O3'-C3'	6.20	127.14	119.70
1	E	5	DT	O4'-C1'-C2'	-6.20	100.94	105.90
1	E	1	DA	O4'-C1'-N9	6.18	112.33	108.00
1	G	12	DT	C5-C4-O4	-6.16	120.59	124.90
1	C	4	DA	P-O3'-C3'	6.15	127.08	119.70
1	A	2	DG	P-O3'-C3'	6.14	127.06	119.70
1	G	5	DT	C3'-C2'-C1'	-6.12	95.15	102.50
1	C	11	DA	O4'-C1'-N9	-6.10	103.73	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	4	DT	C5-C4-O4	-6.09	120.63	124.90
1	A	9	DT	O4'-C1'-N1	-6.09	103.74	108.00
2	B	10	DA	O4'-C1'-N9	-6.03	103.78	108.00
1	E	2	DG	C3'-C2'-C1'	-6.02	95.27	102.50
1	G	12	DT	O4'-C1'-C2'	-6.00	101.10	105.90
1	G	7	DA	O4'-C1'-N9	-5.96	103.83	108.00
2	F	11	DT	C5-C4-O4	-5.95	120.74	124.90
1	E	13	DA	O4'-C1'-N9	-5.94	103.84	108.00
2	H	5	DT	O4'-C1'-N1	-5.94	103.84	108.00
2	D	1	DT	C5-C4-O4	-5.93	120.75	124.90
1	A	13	DA	O4'-C1'-N9	-5.89	103.88	108.00
2	B	1	DT	O4'-C1'-N1	-5.86	103.90	108.00
2	D	6	DA	O4'-C1'-N9	-5.82	103.92	108.00
2	D	3	DA	O4'-C1'-N9	-5.81	103.93	108.00
2	D	9	DT	P-O3'-C3'	5.80	126.67	119.70
2	B	5	DT	O4'-C1'-N1	-5.79	103.95	108.00
1	A	10	DA	O4'-C1'-N9	-5.74	103.98	108.00
1	G	9	DT	O4'-C1'-N1	-5.70	104.01	108.00
2	F	9	DT	C5-C4-O4	-5.69	120.92	124.90
2	B	7	DT	N3-C4-O4	5.68	123.31	119.90
1	C	9	DT	N3-C4-O4	5.68	123.31	119.90
2	F	10	DA	C4'-C3'-C2'	-5.63	98.03	103.10
2	B	1	DT	P-O3'-C3'	-5.63	112.94	119.70
2	F	7	DT	O4'-C1'-N1	-5.62	104.07	108.00
2	B	9	DT	O4'-C1'-N1	-5.61	104.07	108.00
1	A	3	DC	O4'-C1'-N1	-5.61	104.08	108.00
1	G	13	DA	O4'-C1'-N9	-5.59	104.09	108.00
1	E	2	DG	P-O3'-C3'	5.57	126.38	119.70
2	B	13	DC	C4'-C3'-C2'	-5.55	98.10	103.10
2	B	5	DT	C5-C4-O4	-5.53	121.03	124.90
1	A	12	DT	N3-C4-O4	5.49	123.19	119.90
1	E	12	DT	C5-C4-O4	-5.47	121.07	124.90
2	F	14	DT	C1'-O4'-C4'	-5.45	104.65	110.10
2	H	1	DT	N3-C4-O4	5.41	123.15	119.90
2	F	5	DT	C6-C5-C7	-5.35	119.69	122.90
2	B	11	DT	N3-C4-O4	5.33	123.10	119.90
2	F	6	DA	O4'-C1'-N9	-5.33	104.27	108.00
1	A	10	DA	P-O5'-C5'	-5.32	112.38	120.90
1	E	1	DA	O4'-C1'-C2'	-5.32	101.65	105.90
2	F	11	DT	N3-C4-O4	5.30	123.08	119.90
1	E	13	DA	O4'-C1'-C2'	-5.27	101.68	105.90
1	G	3	DC	O4'-C1'-N1	-5.27	104.31	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1	DT	P-O3'-C3'	-5.27	113.38	119.70
2	F	7	DT	C5-C4-O4	-5.24	121.23	124.90
1	C	9	DT	C5-C4-O4	-5.23	121.24	124.90
2	B	11	DT	C4'-C3'-C2'	-5.22	98.40	103.10
2	B	8	DT	O4'-C1'-N1	-5.21	104.35	108.00
2	F	7	DT	N3-C4-O4	5.14	122.98	119.90
1	E	2	DG	O5'-P-OP2	-5.13	101.08	105.70
2	F	8	DT	C5-C4-O4	-5.10	121.33	124.90
1	C	5	DT	C3'-C2'-C1'	-5.08	96.41	102.50
2	F	9	DT	P-O3'-C3'	5.06	125.77	119.70
2	D	4	DT	N3-C4-O4	5.03	122.92	119.90
1	A	12	DT	P-O3'-C3'	5.02	125.72	119.70
2	H	1	DT	C5-C4-O4	-5.01	121.39	124.90

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	287	0	159	13	0
1	C	287	0	159	7	0
1	E	287	0	159	8	0
1	G	287	0	159	8	0
2	B	281	0	165	14	0
2	D	281	0	165	18	0
2	F	281	0	165	21	0
2	H	281	0	165	11	0
3	I	1192	0	1174	65	0
3	J	666	0	654	28	0
3	K	1100	0	1017	68	0
3	L	1130	0	1090	62	0
3	M	1188	0	1157	81	0
3	N	658	0	643	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	O	1166	0	1120	80	0
3	P	620	0	606	22	0
4	A	9	0	0	5	0
4	B	10	0	0	2	0
4	C	5	0	0	0	0
4	D	1	0	0	0	0
4	E	9	0	0	2	0
4	F	10	0	0	3	0
4	G	4	0	0	0	0
4	H	5	0	0	0	0
4	I	8	0	0	2	0
4	J	6	0	0	1	0
4	L	1	0	0	0	0
4	M	10	0	0	1	0
4	N	6	0	0	2	0
4	O	10	0	0	0	0
4	P	3	0	0	1	0
All	All	10089	0	8757	512	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 28.

All (512) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:L:265:THR:HG22	3:L:275:ARG:HE	1.09	1.15
3:L:238:ARG:HG2	3:L:238:ARG:HH11	1.03	1.15
3:M:238:ARG:HH11	3:M:238:ARG:HG2	1.18	1.06
3:K:250:ASN:HA	3:K:253:PHE:HB3	1.38	1.03
2:F:9:DT:OP2	3:N:166:THR:HG23	1.59	1.03
3:O:215:ARG:HG3	3:O:215:ARG:NH1	1.68	1.03
3:O:215:ARG:HG3	3:O:215:ARG:HH11	0.87	1.00
1:G:3:DC:H2''	1:G:4:DA:H5'	1.41	0.99
3:L:215:ARG:HG2	3:L:215:ARG:HH11	1.26	0.98
3:L:265:THR:HG22	3:L:275:ARG:NE	1.79	0.98
3:L:215:ARG:CG	3:L:215:ARG:HH11	1.76	0.98
3:O:215:ARG:CG	3:O:215:ARG:HH11	1.75	0.98
3:O:264:ILE:HA	3:O:267:MSE:HE3	1.42	0.96
1:G:7:DA:OP1	3:O:239:THR:HG23	1.67	0.94
3:M:215:ARG:HG2	3:M:226:PHE:HB2	1.48	0.94
2:D:1:DT:H5'	2:D:1:DT:H6	1.29	0.94
3:M:238:ARG:HH11	3:M:238:ARG:CG	1.81	0.93
2:F:3:DA:H8	4:F:18:HOH:O	1.53	0.91

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:L:238:ARG:HH11	3:L:238:ARG:CG	1.84	0.90
2:B:9:DT:OP2	3:J:166:THR:HG23	1.72	0.88
2:D:9:DT:H2'	2:D:10:DA:C8	2.08	0.88
3:L:238:ARG:HG2	3:L:238:ARG:NH1	1.84	0.88
3:I:237:ARG:HH11	3:I:237:ARG:HB3	1.40	0.87
3:O:157:ARG:HH11	3:O:209:LEU:HD23	1.36	0.87
2:D:1:DT:H2'	2:D:2:DT:C6	2.10	0.86
3:K:150:PHE:HE1	3:K:206:GLU:HG3	1.37	0.85
3:L:157:ARG:NE	3:L:209:LEU:HD13	1.93	0.84
3:L:239:THR:HG22	3:L:274:ASP:HB2	1.60	0.84
3:O:202:LYS:HB3	3:O:203:PRO:HD3	1.59	0.84
3:J:166:THR:HG22	3:J:182:GLN:HG3	1.59	0.83
3:O:169:GLY:O	3:O:173:THR:HG22	1.79	0.83
3:I:194:THR:HG22	3:I:197:SER:H	1.41	0.83
3:P:157:ARG:HH21	3:P:209:LEU:HD22	1.43	0.82
3:O:194:THR:HG22	3:O:196:LYS:H	1.43	0.82
2:B:1:DT:H2'	2:B:2:DT:C6	2.15	0.81
3:O:249:LEU:HD13	3:O:281:TRP:NE1	1.96	0.81
3:O:157:ARG:NH1	3:O:209:LEU:HD23	1.95	0.80
3:N:175:THR:HG23	3:N:176:GLU:HG3	1.62	0.80
3:I:173:THR:HB	3:I:180:TYR:H	1.44	0.80
3:N:216:ASN:HB2	3:N:223:LEU:HG	1.64	0.78
2:H:9:DT:OP2	3:P:166:THR:HG23	1.84	0.78
3:I:202:LYS:HB3	3:I:203:PRO:HD3	1.65	0.78
1:A:2:DG:H5'	3:J:178:PRO:HB2	1.66	0.77
3:I:157:ARG:HD2	3:I:209:LEU:HD21	1.65	0.77
3:N:172:MSE:HE2	3:N:208:TRP:HB3	1.65	0.76
3:M:194:THR:HG22	3:M:197:SER:H	1.49	0.76
3:I:147:ILE:HG22	3:I:202:LYS:HG3	1.68	0.76
3:I:157:ARG:HD3	3:I:213:GLU:OE2	1.85	0.76
1:G:11:DA:OP1	3:O:190:LYS:HE3	1.86	0.75
3:O:259:PRO:HB2	3:O:264:ILE:HG13	1.68	0.75
3:J:145:GLU:CD	3:J:145:GLU:H	1.86	0.75
1:A:2:DG:H8	4:J:12:HOH:O	1.70	0.74
3:I:237:ARG:HB3	3:I:237:ARG:NH1	2.02	0.74
3:I:173:THR:HB	3:I:179:ALA:HA	1.69	0.74
1:A:11:DA:OP1	3:I:190:LYS:HE3	1.88	0.74
3:L:215:ARG:NH1	3:L:215:ARG:HG2	1.96	0.74
3:N:166:THR:HG22	3:N:182:GLN:HG3	1.69	0.73
3:M:238:ARG:CG	3:M:238:ARG:NH1	2.47	0.73
2:D:9:DT:H2''	2:D:10:DA:O5'	1.88	0.73
3:L:157:ARG:CZ	3:L:209:LEU:HD13	2.18	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:1:DT:H2'	2:H:2:DT:C6	2.24	0.73
3:J:175:THR:HG22	3:J:176:GLU:HG2	1.70	0.72
2:D:1:DT:C6	2:D:1:DT:H5'	2.21	0.72
2:F:1:DT:H2''	2:F:2:DT:H5'	1.68	0.72
3:O:194:THR:HB	3:O:197:SER:OG	1.89	0.72
3:N:164:THR:OG1	3:N:167:GLN:HG3	1.88	0.72
1:G:5:DT:O2	3:O:238:ARG:NH2	2.21	0.72
3:O:249:LEU:HD13	3:O:281:TRP:CE2	2.24	0.71
3:O:276:GLU:O	3:O:280:VAL:HG23	1.89	0.71
3:J:172:MSE:HB3	3:J:180:TYR:HB3	1.73	0.71
3:J:181:SER:O	3:J:185:ILE:HG12	1.91	0.70
3:K:224:MSE:HE1	3:K:231:PRO:HB2	1.74	0.70
3:P:175:THR:HG23	3:P:176:GLU:HG2	1.74	0.70
1:E:4:DA:H8	4:E:17:HOH:O	1.73	0.70
3:O:249:LEU:HD22	3:O:281:TRP:CE3	2.27	0.70
3:K:150:PHE:CE1	3:K:206:GLU:HG3	2.24	0.70
3:M:285:ARG:NH1	3:M:289:LEU:HD23	2.08	0.69
3:M:148:ARG:O	3:M:152:LYS:HD3	1.94	0.68
3:M:148:ARG:HA	3:M:191:LEU:HD11	1.75	0.68
3:O:285:ARG:NH1	3:O:289:LEU:HD21	2.09	0.68
2:D:11:DT:OP2	3:L:190:LYS:HE3	1.93	0.68
3:O:249:LEU:HD22	3:O:281:TRP:CD2	2.30	0.67
3:O:249:LEU:HD13	3:O:281:TRP:CD1	2.29	0.67
3:K:216:ASN:O	3:K:223:LEU:HB2	1.95	0.67
3:J:157:ARG:CZ	3:J:209:LEU:HD13	2.25	0.66
3:N:172:MSE:HE2	3:N:208:TRP:CB	2.26	0.66
3:M:285:ARG:NH1	3:M:289:LEU:CD2	2.58	0.66
3:N:187:ARG:CG	3:N:192:ASP:HB3	2.26	0.66
3:L:218:GLU:O	3:L:218:GLU:HG2	1.95	0.66
3:L:157:ARG:HE	3:L:209:LEU:HD13	1.59	0.65
1:C:4:DA:H2''	1:C:5:DT:O5'	1.95	0.65
3:O:145:GLU:H	3:O:145:GLU:CD	2.00	0.65
1:A:2:DG:H2''	1:A:3:DC:O5'	1.97	0.64
2:H:9:DT:H2''	2:H:10:DA:O5'	1.98	0.64
3:O:264:ILE:HA	3:O:267:MSE:CE	2.21	0.64
3:N:187:ARG:HG3	3:N:192:ASP:HB3	1.80	0.64
3:K:144:MSE:HB3	3:K:148:ARG:HH12	1.63	0.64
3:L:148:ARG:HA	3:L:191:LEU:HD11	1.79	0.64
1:G:3:DC:C2'	1:G:4:DA:H5'	2.22	0.64
2:B:7:DT:H2'	4:B:79:HOH:O	1.98	0.64
3:K:264:ILE:HA	3:K:267:MSE:HE3	1.80	0.64
3:J:172:MSE:CB	3:J:180:TYR:HB3	2.28	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:11:DA:H2''	1:C:12:DT:O5'	1.97	0.63
3:I:260:THR:H	3:I:263:GLU:HG3	1.63	0.63
3:O:194:THR:HG22	3:O:196:LYS:N	2.12	0.63
3:N:200:LYS:O	3:N:203:PRO:HD2	1.99	0.63
3:N:187:ARG:HD2	4:N:26:HOH:O	1.99	0.63
3:I:259:PRO:HB2	3:I:264:ILE:HG13	1.80	0.63
3:N:172:MSE:HE2	3:N:208:TRP:CG	2.33	0.63
3:O:144:MSE:SE	3:O:147:ILE:HD11	2.49	0.62
1:A:7:DA:OP1	3:I:239:THR:HG23	1.99	0.62
2:B:12:DG:H1'	2:B:13:DC:H5''	1.82	0.62
3:M:215:ARG:HB3	3:M:223:LEU:HA	1.79	0.62
3:I:260:THR:N	3:I:263:GLU:HG3	2.15	0.62
2:F:11:DT:OP2	3:N:190:LYS:HE3	1.99	0.62
3:M:193:ILE:HD11	3:M:198:ALA:HA	1.80	0.61
3:M:275:ARG:HG3	3:M:275:ARG:HH11	1.65	0.61
3:I:264:ILE:HA	3:I:267:MSE:HE3	1.81	0.61
3:P:173:THR:HA	3:P:177:GLY:O	1.99	0.61
3:I:145:GLU:H	3:I:145:GLU:CD	2.04	0.61
3:O:249:LEU:HB3	3:O:281:TRP:CZ2	2.35	0.61
3:I:157:ARG:HD2	3:I:209:LEU:CD2	2.31	0.61
3:N:163:LEU:HA	3:N:167:GLN:OE1	2.01	0.61
3:N:215:ARG:O	3:N:218:GLU:HB3	2.00	0.61
3:M:238:ARG:NH1	3:M:238:ARG:HG2	2.01	0.61
2:D:9:DT:H3'	3:L:165:GLN:OE1	2.00	0.60
3:I:231:PRO:O	3:I:232:SER:HB3	2.01	0.60
2:F:9:DT:H2''	2:F:10:DA:C5'	2.32	0.60
3:O:154:PHE:CD1	3:O:209:LEU:HD22	2.37	0.60
3:K:212:ALA:HB2	3:K:226:PHE:CE2	2.37	0.60
3:M:243:PRO:O	3:M:246:ILE:HG22	2.02	0.60
3:J:180:TYR:CE2	3:J:201:LEU:HD22	2.36	0.60
3:L:157:ARG:NH2	3:L:209:LEU:HD13	2.16	0.59
3:J:218:GLU:HG2	3:J:222:ASN:OD1	2.02	0.59
3:M:231:PRO:CA	3:M:232:SER:HB3	2.32	0.59
3:O:241:PHE:CE1	3:O:281:TRP:HD1	2.20	0.59
3:K:243:PRO:HA	3:K:246:ILE:HB	1.82	0.59
3:I:144:MSE:SE	3:I:147:ILE:HD11	2.53	0.59
3:K:284:ASN:O	3:K:288:THR:HG23	2.01	0.59
3:I:195:PRO:O	3:I:199:GLN:HG3	2.01	0.59
3:K:257:PRO:O	3:K:259:PRO:HD3	2.03	0.59
2:F:9:DT:OP2	3:N:166:THR:CG2	2.44	0.59
3:K:157:ARG:HH11	3:K:209:LEU:HD21	1.68	0.59
3:M:248:ALA:O	3:M:251:ALA:HB3	2.03	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:9:DT:C2'	2:D:10:DA:C8	2.85	0.58
3:O:157:ARG:HH11	3:O:209:LEU:CD2	2.11	0.58
3:L:265:THR:CG2	3:L:275:ARG:HE	2.01	0.58
2:D:9:DT:H5'	2:D:9:DT:H6	1.69	0.58
3:N:215:ARG:HG3	3:N:226:PHE:CG	2.38	0.58
3:O:285:ARG:CZ	3:O:289:LEU:HD21	2.33	0.58
3:M:202:LYS:HB3	3:M:203:PRO:HD3	1.85	0.58
2:D:1:DT:H2''	2:D:2:DT:O5'	2.04	0.58
3:M:194:THR:HB	3:M:197:SER:OG	2.04	0.58
1:A:4:DA:H8	4:A:16:HOH:O	1.87	0.58
2:H:9:DT:H4'	2:H:10:DA:OP1	2.04	0.58
2:F:9:DT:H1'	2:F:10:DA:H5''	1.85	0.57
3:M:175:THR:HB	3:M:176:GLU:HG2	1.84	0.57
3:K:250:ASN:HA	3:K:253:PHE:CB	2.24	0.57
3:I:173:THR:HB	3:I:180:TYR:N	2.17	0.57
2:F:8:DT:H2''	2:F:9:DT:O5'	2.04	0.57
3:L:157:ARG:NH2	3:L:209:LEU:HB3	2.19	0.57
3:K:167:GLN:HA	3:K:170:GLN:HE21	1.68	0.57
1:G:10:DA:C2	2:H:6:DA:C2	2.92	0.57
1:E:7:DA:OP1	3:M:239:THR:CG2	2.52	0.57
3:M:260:THR:H	3:M:263:GLU:CG	2.18	0.57
3:O:259:PRO:HB2	3:O:264:ILE:CG1	2.35	0.57
2:D:2:DT:H2''	2:D:3:DA:O5'	2.05	0.57
1:E:7:DA:OP1	3:M:239:THR:HG23	2.06	0.56
3:N:222:ASN:N	3:N:222:ASN:HD22	2.04	0.56
1:E:7:DA:P	3:M:239:THR:HG23	2.46	0.56
3:K:183:SER:O	3:K:187:ARG:HG2	2.05	0.56
1:A:5:DT:O2	3:I:238:ARG:NH2	2.35	0.56
3:L:253:PHE:CZ	3:L:285:ARG:HG3	2.40	0.56
3:M:231:PRO:HA	3:M:232:SER:HB3	1.87	0.56
3:M:260:THR:OG1	3:M:263:GLU:HG2	2.04	0.56
3:K:247:GLU:HA	3:K:250:ASN:HD21	1.71	0.56
2:B:9:DT:H2''	2:B:10:DA:C8	2.41	0.56
3:L:168:VAL:HG12	3:L:172:MSE:HG3	1.86	0.56
3:K:174:ALA:N	3:K:175:THR:HA	2.20	0.56
3:J:148:ARG:HA	3:J:191:LEU:HD11	1.86	0.56
1:A:5:DT:H6	4:A:15:HOH:O	1.89	0.56
3:O:181:SER:O	3:O:185:ILE:HG12	2.05	0.56
2:F:1:DT:H2'	2:F:2:DT:C6	2.40	0.56
3:P:202:LYS:HB3	3:P:203:PRO:HD3	1.88	0.56
3:K:225:GLU:HA	3:K:225:GLU:OE1	2.05	0.55
3:I:169:GLY:O	3:I:173:THR:HG22	2.05	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:P:157:ARG:O	3:P:161:LEU:HD13	2.06	0.55
3:P:190:LYS:HD3	4:P:62:HOH:O	2.05	0.55
3:I:260:THR:H	3:I:263:GLU:CG	2.19	0.55
3:M:231:PRO:HB3	3:M:232:SER:HB3	1.87	0.55
3:O:157:ARG:NH1	3:O:209:LEU:CD2	2.67	0.55
3:K:157:ARG:HD3	3:K:213:GLU:OE2	2.06	0.54
2:B:11:DT:OP2	3:J:190:LYS:HE3	2.07	0.54
3:M:169:GLY:O	3:M:173:THR:HG23	2.07	0.54
3:L:261:GLY:O	3:L:265:THR:HG23	2.06	0.54
3:J:164:THR:OG1	3:J:167:GLN:HG3	2.07	0.54
3:O:172:MSE:HE1	3:O:205:LEU:HA	1.89	0.54
3:I:236:LYS:NZ	3:I:236:LYS:HB3	2.22	0.54
3:I:157:ARG:NH1	3:I:209:LEU:HD23	2.22	0.54
3:M:173:THR:HB	3:M:179:ALA:HA	1.88	0.54
3:M:194:THR:HG22	3:M:196:LYS:N	2.23	0.54
3:O:211:GLU:O	3:O:215:ARG:HG2	2.07	0.54
3:M:215:ARG:HE	3:M:215:ARG:HA	1.72	0.54
3:I:149:GLU:OE2	3:I:149:GLU:HA	2.08	0.54
3:M:231:PRO:CB	3:M:232:SER:HB3	2.38	0.54
2:F:3:DA:C8	4:F:18:HOH:O	2.39	0.54
1:C:10:DA:H2'	3:K:165:GLN:OE1	2.08	0.53
3:O:190:LYS:O	3:O:191:LEU:HB2	2.08	0.53
3:M:147:ILE:HG22	3:M:202:LYS:HG3	1.89	0.53
1:E:12:DT:O4	3:M:183:SER:OG	2.26	0.53
3:L:156:ILE:HG22	3:L:157:ARG:N	2.22	0.53
3:P:143:ASN:O	3:P:147:ILE:HG13	2.08	0.53
3:K:202:LYS:HB3	3:K:203:PRO:HD3	1.91	0.53
3:N:175:THR:O	3:N:176:GLU:HG3	2.08	0.53
3:M:276:GLU:OE2	3:M:279:ARG:NH1	2.42	0.53
3:K:216:ASN:C	3:K:223:LEU:HB2	2.29	0.53
3:M:230:GLU:N	3:M:231:PRO:HD3	2.24	0.53
3:K:157:ARG:HD2	3:K:209:LEU:HD21	1.91	0.53
3:M:173:THR:CG2	3:M:180:TYR:H	2.22	0.52
3:L:228:GLY:N	3:L:229:GLY:HA2	2.24	0.52
3:L:237:ARG:NH2	3:L:269:LYS:HA	2.24	0.52
3:N:157:ARG:O	3:N:161:LEU:HD13	2.08	0.52
3:L:187:ARG:HG2	3:L:192:ASP:HB3	1.91	0.52
3:K:188:PHE:CZ	3:K:205:LEU:HD12	2.44	0.52
3:K:147:ILE:HG22	3:K:202:LYS:HG3	1.92	0.52
3:M:244:GLN:O	3:M:247:GLU:HB3	2.10	0.52
3:K:152:LYS:N	3:K:152:LYS:HD2	2.23	0.52
3:I:284:ASN:HA	3:I:287:GLN:NE2	2.23	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:M:276:GLU:O	3:M:280:VAL:HG23	2.10	0.52
3:K:292:THR:HA	3:L:235:ARG:HG3	1.91	0.52
2:F:9:DT:H2''	2:F:10:DA:H5'	1.90	0.52
3:K:230:GLU:N	3:K:231:PRO:HD3	2.25	0.52
3:O:221:GLN:HA	3:O:221:GLN:NE2	2.23	0.52
3:N:221:GLN:O	3:N:225:GLU:HG3	2.09	0.52
3:M:281:TRP:CH2	3:M:285:ARG:HG3	2.44	0.52
3:L:157:ARG:HH21	3:L:209:LEU:HB3	1.74	0.52
3:M:144:MSE:HB3	3:M:148:ARG:HH12	1.75	0.52
3:N:181:SER:O	3:N:185:ILE:HG12	2.09	0.51
3:I:276:GLU:OE2	3:I:279:ARG:NH1	2.43	0.51
1:E:4:DA:H1'	4:E:22:HOH:O	2.09	0.51
3:O:244:GLN:CD	3:O:244:GLN:H	2.13	0.51
3:I:173:THR:CB	3:I:179:ALA:HA	2.40	0.51
3:N:187:ARG:HG2	3:N:192:ASP:HB3	1.91	0.51
2:H:9:DT:C2'	2:H:10:DA:C8	2.94	0.51
3:K:173:THR:HG23	3:K:175:THR:OG1	2.10	0.51
3:O:243:PRO:O	3:O:246:ILE:HG12	2.10	0.51
3:I:250:ASN:HA	3:I:253:PHE:HB3	1.93	0.51
3:I:264:ILE:HA	3:I:267:MSE:CE	2.40	0.51
3:O:247:GLU:HA	3:O:250:ASN:HD21	1.75	0.51
3:O:255:LYS:O	3:O:257:PRO:HD3	2.11	0.51
3:O:262:GLN:O	3:O:265:THR:HG22	2.10	0.51
3:K:276:GLU:O	3:K:280:VAL:HG23	2.11	0.51
3:P:156:ILE:HG22	3:P:157:ARG:N	2.26	0.51
3:K:217:GLN:OE1	3:K:217:GLN:HA	2.11	0.51
3:N:175:THR:HG23	3:N:176:GLU:CG	2.37	0.51
3:J:187:ARG:HG2	3:J:192:ASP:HB3	1.92	0.51
3:M:193:ILE:HD11	3:M:198:ALA:CA	2.40	0.50
3:K:249:LEU:HD13	3:K:281:TRP:CD1	2.45	0.50
3:L:157:ARG:HE	3:L:209:LEU:CD1	2.24	0.50
3:M:285:ARG:HH12	3:M:289:LEU:HD21	1.77	0.50
3:M:259:PRO:HB3	3:M:263:GLU:HG3	1.92	0.50
3:O:248:ALA:O	3:O:251:ALA:HB3	2.12	0.50
1:C:10:DA:C2	2:D:6:DA:C2	2.99	0.50
3:M:214:LEU:O	3:M:218:GLU:HG3	2.11	0.50
2:H:6:DA:H1'	2:H:7:DT:H5''	1.92	0.50
3:K:212:ALA:HB2	3:K:226:PHE:CZ	2.47	0.50
3:O:173:THR:HB	3:O:180:TYR:H	1.77	0.50
3:P:158:ARG:NH1	3:P:165:GLN:N	2.59	0.50
3:I:157:ARG:HH11	3:I:209:LEU:HD23	1.75	0.50
3:M:284:ASN:O	3:M:288:THR:HG23	2.11	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:L:219:GLY:C	3:L:221:GLN:H	2.15	0.50
3:L:214:LEU:HD13	3:L:215:ARG:HD2	1.92	0.50
3:P:163:LEU:HA	3:P:167:GLN:OE1	2.12	0.50
2:D:12:DG:H2'	2:D:13:DC:O5'	2.11	0.50
3:O:241:PHE:HB2	3:O:246:ILE:HG22	1.94	0.50
1:A:5:DT:H2'	4:A:15:HOH:O	2.12	0.50
2:H:9:DT:H2'	2:H:10:DA:C8	2.47	0.49
2:H:9:DT:H3'	3:P:165:GLN:OE1	2.11	0.49
3:O:165:GLN:HB3	3:O:182:GLN:HG2	1.94	0.49
3:M:266:GLU:O	3:M:270:GLU:HG2	2.13	0.49
3:P:157:ARG:NH2	3:P:209:LEU:HD22	2.22	0.49
3:N:187:ARG:HG2	3:N:192:ASP:O	2.12	0.49
3:L:237:ARG:HH22	3:L:269:LYS:HA	1.76	0.49
3:I:284:ASN:HA	3:I:287:GLN:HE21	1.77	0.49
3:L:222:ASN:HA	3:L:225:GLU:CD	2.33	0.49
3:L:250:ASN:OD1	3:L:285:ARG:NH2	2.45	0.49
4:A:19:HOH:O	3:I:166:THR:HG22	2.12	0.49
2:B:5:DT:H71	4:B:88:HOH:O	2.11	0.49
3:K:276:GLU:OE2	3:K:276:GLU:HA	2.13	0.49
3:L:145:GLU:O	3:L:149:GLU:HG2	2.12	0.49
3:N:148:ARG:HA	3:N:191:LEU:HD11	1.95	0.49
3:L:172:MSE:HB3	3:L:180:TYR:HB3	1.93	0.49
3:I:158:ARG:HD3	3:I:168:VAL:HG21	1.95	0.49
3:L:155:LYS:HG3	3:L:158:ARG:HH21	1.78	0.49
3:I:220:GLN:O	3:I:224:MSE:HG2	2.13	0.49
3:O:241:PHE:CE1	3:O:281:TRP:CD1	3.01	0.49
3:N:212:ALA:HB2	3:N:226:PHE:HE2	1.78	0.49
3:K:158:ARG:HD2	3:K:163:LEU:O	2.13	0.49
3:I:150:PHE:HE1	3:I:206:GLU:HG3	1.78	0.49
3:P:172:MSE:HA	3:P:175:THR:HG22	1.94	0.48
3:K:206:GLU:C	3:K:208:TRP:H	2.17	0.48
3:K:145:GLU:HA	3:K:148:ARG:HB3	1.95	0.48
1:A:9:DT:H1'	1:A:10:DA:H5'	1.96	0.48
3:L:170:GLN:NE2	3:L:170:GLN:HA	2.29	0.48
3:N:187:ARG:CD	4:N:26:HOH:O	2.60	0.48
3:K:243:PRO:O	3:K:246:ILE:HG22	2.13	0.48
1:G:2:DG:H5'	3:P:178:PRO:HB2	1.96	0.48
2:F:8:DT:H2'	2:F:9:DT:H72	1.94	0.48
3:N:211:GLU:O	3:N:214:LEU:HB3	2.13	0.48
3:I:202:LYS:HB3	3:I:203:PRO:CD	2.41	0.48
3:K:143:ASN:ND2	3:K:146:GLU:HG3	2.29	0.48
3:M:268:ALA:HA	3:M:278:VAL:HG21	1.95	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:L:200:LYS:O	3:L:203:PRO:HD2	2.13	0.48
3:M:275:ARG:HG3	3:M:275:ARG:NH1	2.27	0.48
1:A:8:DA:H2'	4:A:21:HOH:O	2.14	0.48
3:M:157:ARG:NH1	3:M:209:LEU:HD23	2.29	0.48
3:J:200:LYS:O	3:J:203:PRO:HD2	2.13	0.48
3:M:172:MSE:SE	3:M:205:LEU:HD23	2.64	0.48
3:M:177:GLY:HA2	3:M:178:PRO:HA	1.69	0.48
2:D:2:DT:H2''	2:D:3:DA:C5'	2.44	0.47
3:M:191:LEU:HD23	3:M:191:LEU:HA	1.50	0.47
1:C:7:DA:H2''	1:C:8:DA:O5'	2.14	0.47
3:L:215:ARG:HG3	3:L:215:ARG:HH11	1.69	0.47
3:I:202:LYS:CB	3:I:203:PRO:HD3	2.38	0.47
3:I:279:ARG:NE	4:I:92:HOH:O	2.47	0.47
3:I:221:GLN:HA	3:I:224:MSE:HB2	1.97	0.47
3:O:242:THR:O	3:O:246:ILE:HG23	2.14	0.47
3:K:291:ASN:HB3	3:L:235:ARG:HA	1.97	0.47
2:F:9:DT:C2'	2:F:10:DA:H5''	2.45	0.47
3:M:244:GLN:NE2	3:M:244:GLN:H	2.13	0.47
3:I:276:GLU:HA	3:I:276:GLU:OE2	2.14	0.47
3:P:216:ASN:CB	3:P:223:LEU:HD11	2.45	0.47
3:N:223:LEU:O	3:N:226:PHE:HB3	2.15	0.47
3:K:224:MSE:HE1	3:K:231:PRO:CB	2.44	0.47
2:B:11:DT:H2'	2:B:11:DT:O5'	2.15	0.47
2:F:9:DT:H2''	2:F:10:DA:H5''	1.96	0.46
3:M:285:ARG:HD3	3:M:285:ARG:O	2.14	0.46
3:O:285:ARG:O	3:O:285:ARG:HD2	2.15	0.46
3:J:143:ASN:O	3:J:146:GLU:HB3	2.15	0.46
3:O:243:PRO:HD2	3:O:244:GLN:NE2	2.30	0.46
3:N:209:LEU:HA	3:N:209:LEU:HD23	1.70	0.46
2:B:3:DA:C2	2:B:4:DT:C2	3.04	0.46
3:J:172:MSE:HB3	3:J:180:TYR:CB	2.44	0.46
3:M:259:PRO:HA	3:M:263:GLU:OE2	2.16	0.46
3:L:279:ARG:HH11	3:L:279:ARG:CG	2.28	0.46
3:I:194:THR:CG2	3:I:197:SER:H	2.22	0.46
3:K:166:THR:HB	3:K:182:GLN:HG3	1.98	0.46
3:O:157:ARG:NH2	3:O:213:GLU:OE1	2.49	0.46
1:E:13:DA:C2	2:F:3:DA:C2	3.03	0.46
3:M:258:LEU:N	3:M:259:PRO:HD3	2.30	0.46
3:O:143:ASN:O	3:O:147:ILE:HG12	2.16	0.46
3:K:157:ARG:NH1	3:K:209:LEU:HD21	2.31	0.46
3:O:263:GLU:HA	3:O:266:GLU:OE1	2.15	0.46
3:M:215:ARG:HG2	3:M:226:PHE:CB	2.34	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:3:DA:H2'	4:F:18:HOH:O	2.16	0.46
3:M:289:LEU:HA	3:M:289:LEU:HD22	1.69	0.46
3:O:149:GLU:HA	3:O:149:GLU:OE2	2.16	0.46
3:I:266:GLU:O	3:I:269:LYS:HE2	2.15	0.45
1:A:7:DA:OP1	3:I:239:THR:CG2	2.63	0.45
3:M:243:PRO:HD2	3:M:244:GLN:HE22	1.81	0.45
3:L:215:ARG:CG	3:L:215:ARG:NH1	2.47	0.45
3:K:143:ASN:HD21	3:K:146:GLU:HG3	1.81	0.45
3:M:172:MSE:CE	3:M:204:VAL:HG22	2.46	0.45
3:L:256:ASN:C	3:L:256:ASN:HD22	2.18	0.45
3:I:181:SER:O	3:I:185:ILE:HG12	2.17	0.45
3:I:291:ASN:O	3:I:292:THR:HG23	2.17	0.45
3:J:167:GLN:O	3:J:170:GLN:HB3	2.16	0.45
3:N:143:ASN:O	3:N:146:GLU:HB3	2.17	0.45
3:M:144:MSE:O	3:M:145:GLU:C	2.55	0.45
3:K:205:LEU:HD23	3:K:205:LEU:HA	1.67	0.45
3:I:287:GLN:HE21	3:I:287:GLN:HB3	1.65	0.45
3:L:181:SER:O	3:L:185:ILE:HG12	2.16	0.45
2:D:1:DT:H2'	2:D:2:DT:H6	1.72	0.45
1:C:4:DA:H2''	1:C:5:DT:C5'	2.46	0.45
3:O:187:ARG:HD2	3:O:192:ASP:OD1	2.17	0.45
3:O:250:ASN:HA	3:O:253:PHE:HB3	1.99	0.45
3:O:158:ARG:HD2	3:O:163:LEU:O	2.17	0.45
3:M:143:ASN:CG	3:M:146:GLU:HB2	2.37	0.45
3:K:185:ILE:O	3:K:189:GLU:HG3	2.17	0.45
3:L:149:GLU:O	3:L:152:LYS:HB3	2.17	0.45
2:D:9:DT:C6	2:D:9:DT:H5'	2.51	0.45
3:I:157:ARG:HH11	3:I:209:LEU:CD2	2.30	0.45
3:M:172:MSE:HE2	3:M:204:VAL:HG22	1.99	0.44
3:M:187:ARG:NH1	3:M:192:ASP:O	2.50	0.44
3:O:161:LEU:CD2	3:O:223:LEU:HD11	2.47	0.44
3:O:258:LEU:N	3:O:259:PRO:HD3	2.32	0.44
3:O:153:ASN:O	3:O:157:ARG:HB2	2.18	0.44
3:I:263:GLU:HA	3:I:266:GLU:OE1	2.16	0.44
3:O:221:GLN:HA	3:O:221:GLN:HE21	1.82	0.44
3:M:269:LYS:HE2	3:M:269:LYS:HB3	1.51	0.44
3:N:218:GLU:HG2	3:N:222:ASN:OD1	2.17	0.44
3:O:201:LEU:O	3:O:202:LYS:C	2.55	0.44
3:L:235:ARG:HG2	3:L:236:LYS:N	2.33	0.44
3:L:221:GLN:O	3:L:225:GLU:HG3	2.18	0.44
3:O:192:ASP:O	3:O:193:ILE:HG23	2.18	0.44
3:P:168:VAL:CG1	3:P:172:MSE:HE3	2.47	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:M:143:ASN:C	3:M:143:ASN:OD1	2.56	0.44
3:K:260:THR:H	3:K:263:GLU:HG2	1.83	0.44
2:B:5:DT:H2''	2:B:6:DA:H5'	1.99	0.44
3:O:188:PHE:CD1	3:O:188:PHE:C	2.91	0.44
3:K:151:ALA:HB2	3:K:191:LEU:HD21	1.99	0.44
2:F:9:DT:H2''	2:F:10:DA:C8	2.53	0.43
3:P:166:THR:HG22	3:P:182:GLN:HG3	1.99	0.43
3:N:199:GLN:HE21	3:N:199:GLN:HB2	1.67	0.43
3:K:150:PHE:CB	3:K:202:LYS:HE2	2.49	0.43
3:K:170:GLN:O	3:K:173:THR:HG22	2.18	0.43
2:D:4:DT:H2''	2:D:5:DT:O5'	2.18	0.43
3:J:168:VAL:O	3:J:172:MSE:HG2	2.18	0.43
3:K:228:GLY:O	3:K:231:PRO:HG3	2.19	0.43
3:L:285:ARG:HD3	3:L:285:ARG:HA	1.88	0.43
3:J:215:ARG:HG3	3:J:226:PHE:CG	2.54	0.43
3:K:261:GLY:O	3:K:265:THR:HG22	2.18	0.43
3:M:274:ASP:C	3:M:274:ASP:OD1	2.56	0.43
3:J:163:LEU:HA	3:J:167:GLN:OE1	2.17	0.43
3:M:243:PRO:HD2	3:M:244:GLN:NE2	2.33	0.43
3:I:250:ASN:ND2	3:I:250:ASN:H	2.16	0.43
3:I:289:LEU:C	3:I:291:ASN:H	2.20	0.43
3:I:148:ARG:HA	3:I:191:LEU:HD11	2.01	0.43
3:O:230:GLU:HB3	3:O:231:PRO:HD2	2.00	0.43
2:F:10:DA:H5'	2:F:10:DA:C8	2.53	0.43
3:K:159:LEU:C	3:K:161:LEU:H	2.21	0.43
3:O:220:GLN:O	3:O:220:GLN:HG3	2.18	0.43
3:O:201:LEU:HD23	3:O:201:LEU:HA	1.86	0.43
3:O:191:LEU:HA	3:O:191:LEU:HD23	1.59	0.43
1:E:6:DA:O3'	3:M:239:THR:HG23	2.18	0.43
3:K:181:SER:O	3:K:185:ILE:HG12	2.18	0.43
3:J:212:ALA:HB2	3:J:226:PHE:HE2	1.83	0.43
3:L:223:LEU:HD23	3:L:223:LEU:HA	1.78	0.43
3:L:230:GLU:H	3:L:231:PRO:HD3	1.82	0.43
3:M:238:ARG:NH1	4:M:5:HOH:O	2.51	0.43
1:C:13:DA:H1'	1:C:14:DA:H5''	2.00	0.43
3:K:208:TRP:CE2	3:K:226:PHE:HE2	2.37	0.43
3:I:143:ASN:ND2	3:I:146:GLU:HG2	2.34	0.43
3:N:167:GLN:O	3:N:170:GLN:HB3	2.19	0.43
3:P:172:MSE:HA	3:P:175:THR:CG2	2.48	0.43
3:L:222:ASN:HA	3:L:225:GLU:HG3	2.01	0.43
2:H:14:DT:H6	2:H:14:DT:H2'	1.47	0.43
3:K:173:THR:OG1	3:K:175:THR:HG23	2.18	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:L:162:GLY:O	3:L:163:LEU:HD23	2.19	0.42
3:O:209:LEU:HA	3:O:209:LEU:HD12	1.59	0.42
3:M:152:LYS:N	3:M:152:LYS:HD2	2.34	0.42
3:M:147:ILE:H	3:M:147:ILE:HG12	1.55	0.42
2:B:11:DT:O4	3:J:183:SER:HB2	2.19	0.42
3:N:175:THR:C	3:N:176:GLU:HG3	2.40	0.42
3:N:173:THR:HG23	3:N:180:TYR:C	2.40	0.42
3:N:157:ARG:CZ	3:N:209:LEU:HD13	2.50	0.42
3:L:170:GLN:HE21	3:L:170:GLN:HA	1.83	0.42
3:O:241:PHE:HA	3:O:273:TYR:OH	2.20	0.42
3:N:202:LYS:HB3	3:N:203:PRO:HD3	2.00	0.42
3:I:250:ASN:O	3:I:254:GLU:HG2	2.20	0.42
3:K:249:LEU:HD13	3:K:281:TRP:CE2	2.54	0.42
3:L:279:ARG:CG	3:L:279:ARG:NH1	2.81	0.42
3:I:262:GLN:O	3:I:265:THR:HG22	2.20	0.42
3:O:259:PRO:HB3	3:O:263:GLU:HG3	2.00	0.42
3:O:202:LYS:HB3	3:O:203:PRO:CD	2.42	0.42
3:M:194:THR:HG22	3:M:197:SER:N	2.26	0.42
3:O:247:GLU:HA	3:O:250:ASN:ND2	2.35	0.42
2:D:14:DT:H2'	2:D:14:DT:H6	1.57	0.42
3:I:229:GLY:O	3:I:230:GLU:O	2.37	0.42
3:O:215:ARG:HA	3:O:215:ARG:HD2	1.82	0.42
3:O:285:ARG:O	3:O:289:LEU:HD23	2.19	0.42
3:K:223:LEU:C	3:K:223:LEU:HD13	2.41	0.42
3:M:243:PRO:HA	3:M:246:ILE:HG22	2.00	0.42
3:L:222:ASN:HA	3:L:225:GLU:CG	2.50	0.42
2:B:2:DT:H1'	2:B:3:DA:H5'	2.02	0.41
2:F:1:DT:H2''	2:F:2:DT:C5'	2.45	0.41
3:J:172:MSE:HE3	3:J:205:LEU:CD2	2.50	0.41
3:O:289:LEU:HD13	3:O:289:LEU:HA	1.78	0.41
3:L:191:LEU:HA	3:L:191:LEU:HD23	1.77	0.41
1:A:7:DA:P	3:I:239:THR:HG23	2.60	0.41
3:O:253:PHE:HD1	3:O:282:PHE:CD2	2.38	0.41
3:M:158:ARG:HD2	3:M:163:LEU:O	2.20	0.41
3:M:231:PRO:CA	3:M:232:SER:CB	2.99	0.41
3:M:173:THR:HG22	3:M:180:TYR:H	1.84	0.41
3:K:236:LYS:HZ2	3:K:236:LYS:HB3	1.85	0.41
3:K:237:ARG:CZ	3:K:237:ARG:HB3	2.49	0.41
3:I:239:THR:HA	4:I:61:HOH:O	2.20	0.41
2:F:14:DT:H2'	2:F:14:DT:H6	1.40	0.41
3:L:149:GLU:HA	3:L:149:GLU:OE2	2.21	0.41
3:O:215:ARG:CG	3:O:215:ARG:NH1	2.46	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:P:157:ARG:CZ	3:P:209:LEU:HD13	2.50	0.41
3:O:285:ARG:NH1	3:O:289:LEU:CD2	2.81	0.41
2:H:10:DA:OP2	3:P:190:LYS:HD2	2.21	0.41
3:L:235:ARG:HE	3:L:235:ARG:HB3	1.72	0.41
3:K:148:ARG:NH1	3:K:148:ARG:HB2	2.36	0.41
3:O:280:VAL:O	3:O:284:ASN:HB2	2.21	0.41
3:M:274:ASP:O	3:M:277:VAL:HB	2.21	0.41
3:J:201:LEU:HA	3:J:201:LEU:HD23	1.84	0.41
2:B:12:DG:C2'	2:B:13:DC:H5''	2.51	0.41
3:K:163:LEU:HD23	3:K:167:GLN:OE1	2.20	0.41
3:M:173:THR:HG22	3:M:180:TYR:HB2	2.03	0.41
3:I:251:ALA:O	3:I:254:GLU:HB2	2.21	0.41
3:L:256:ASN:C	3:L:256:ASN:ND2	2.74	0.41
3:K:271:LEU:HD23	3:K:271:LEU:HA	1.88	0.41
3:I:249:LEU:HD23	3:I:249:LEU:HA	1.91	0.41
3:L:252:TYR:CE1	3:L:267:MSE:HG2	2.56	0.41
3:I:223:LEU:O	3:I:226:PHE:HB3	2.20	0.41
3:K:185:ILE:HG12	3:K:185:ILE:H	1.59	0.40
2:B:9:DT:OP2	3:J:164:THR:HB	2.22	0.40
3:K:255:LYS:O	3:K:257:PRO:HD3	2.21	0.40
3:M:215:ARG:NE	3:M:215:ARG:HA	2.35	0.40
3:K:280:VAL:HA	3:K:283:SER:HB2	2.03	0.40
3:K:247:GLU:HA	3:K:250:ASN:ND2	2.36	0.40
2:F:3:DA:H1'	2:F:4:DT:H5'	2.03	0.40
3:K:150:PHE:HE1	3:K:206:GLU:CG	2.20	0.40
3:L:157:ARG:O	3:L:161:LEU:HD13	2.22	0.40
3:P:144:MSE:SE	3:P:147:ILE:HD12	2.71	0.40
3:I:170:GLN:HE21	3:I:170:GLN:HB3	1.67	0.40
3:I:173:THR:O	3:I:173:THR:HG23	2.21	0.40
3:M:279:ARG:HH11	3:M:279:ARG:HD3	1.71	0.40
3:J:202:LYS:N	3:J:203:PRO:CD	2.85	0.40
1:G:8:DA:C2	1:G:9:DT:C2	3.09	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	I	148/151 (98%)	123 (83%)	17 (12%)	8 (5%)	3	2
3	J	84/151 (56%)	78 (93%)	6 (7%)	0	100	100
3	K	148/151 (98%)	119 (80%)	22 (15%)	7 (5%)	4	3
3	L	143/151 (95%)	122 (85%)	16 (11%)	5 (4%)	6	7
3	M	148/151 (98%)	136 (92%)	10 (7%)	2 (1%)	16	27
3	N	83/151 (55%)	79 (95%)	3 (4%)	1 (1%)	19	32
3	O	148/151 (98%)	127 (86%)	19 (13%)	2 (1%)	16	27
3	P	80/151 (53%)	70 (88%)	9 (11%)	1 (1%)	18	29
All	All	982/1208 (81%)	854 (87%)	102 (10%)	26 (3%)	8	11

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	I	230	GLU
3	I	231	PRO
3	I	232	SER
3	K	218	GLU
3	N	218	GLU
3	I	218	GLU
3	I	229	GLY
3	K	168	VAL
3	L	219	GLY
3	L	228	GLY
3	M	232	SER
3	I	161	LEU
3	I	255	LYS
3	K	232	SER
3	I	290	LYS
3	M	176	GLU
3	K	207	LYS
3	K	231	PRO
3	O	251	ALA
3	P	156	ILE
3	K	249	LEU
3	L	220	GLN
3	O	161	LEU
3	K	219	GLY

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Mol	Chain	Res	Type
3	L	156	ILE
3	L	230	GLU

### 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	I	125/129 (97%)	103 (82%)	22 (18%)	3	4
3	J	69/129 (54%)	63 (91%)	6 (9%)	15	27
3	K	105/129 (81%)	89 (85%)	16 (15%)	4	7
3	L	115/129 (89%)	105 (91%)	10 (9%)	15	27
3	M	124/129 (96%)	96 (77%)	28 (23%)	1	2
3	N	68/129 (53%)	63 (93%)	5 (7%)	20	35
3	O	119/129 (92%)	98 (82%)	21 (18%)	3	4
3	P	62/129 (48%)	56 (90%)	6 (10%)	12	21
All	All	787/1032 (76%)	673 (86%)	114 (14%)	5	8

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	I	158	ARG
3	I	161	LEU
3	I	166	THR
3	I	170	GLN
3	I	172	MSE
3	I	194	THR
3	I	204	VAL
3	I	214	LEU
3	I	215	ARG
3	I	220	GLN
3	I	236	LYS
3	I	239	THR
3	I	247	GLU
3	I	250	ASN
3	I	258	LEU

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Mol	Chain	Res	Type
3	I	263	GLU
3	I	265	THR
3	I	269	LYS
3	I	285	ARG
3	I	287	GLN
3	I	289	LEU
3	I	292	THR
3	J	145	GLU
3	J	149	GLU
3	J	161	LEU
3	J	170	GLN
3	J	209	LEU
3	J	223	LEU
3	K	146	GLU
3	K	152	LYS
3	K	161	LEU
3	K	166	THR
3	K	170	GLN
3	K	194	THR
3	K	214	LEU
3	K	218	GLU
3	K	223	LEU
3	K	225	GLU
3	K	232	SER
3	K	236	LYS
3	K	237	ARG
3	K	250	ASN
3	K	274	ASP
3	K	279	ARG
3	L	176	GLU
3	L	209	LEU
3	L	215	ARG
3	L	221	GLN
3	L	224	MSE
3	L	238	ARG
3	L	256	ASN
3	L	279	ARG
3	L	283	SER
3	L	286	ARG
3	M	146	GLU
3	M	147	ILE
3	M	166	THR

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Mol	Chain	Res	Type
3	M	170	GLN
3	M	173	THR
3	M	175	THR
3	M	183	SER
3	M	190	LYS
3	M	194	THR
3	M	197	SER
3	M	211	GLU
3	M	215	ARG
3	M	220	GLN
3	M	223	LEU
3	M	225	GLU
3	M	238	ARG
3	M	239	THR
3	M	240	SER
3	M	244	GLN
3	M	247	GLU
3	M	258	LEU
3	M	269	LYS
3	M	270	GLU
3	M	274	ASP
3	M	283	SER
3	M	285	ARG
3	M	287	GLN
3	M	289	LEU
3	N	173	THR
3	N	187	ARG
3	N	199	GLN
3	N	222	ASN
3	N	223	LEU
3	O	147	ILE
3	O	157	ARG
3	O	161	LEU
3	O	166	THR
3	O	170	GLN
3	O	173	THR
3	O	175	THR
3	O	197	SER
3	O	215	ARG
3	O	218	GLU
3	O	223	LEU
3	O	225	GLU

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Mol	Chain	Res	Type
3	O	232	SER
3	O	235	ARG
3	O	244	GLN
3	O	246	ILE
3	O	250	ASN
3	O	258	LEU
3	O	269	LYS
3	O	285	ARG
3	O	287	GLN
3	P	147	ILE
3	P	155	LYS
3	P	209	LEU
3	P	214	LEU
3	P	223	LEU
3	P	224	MSE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
3	I	170	GLN
3	I	220	GLN
3	I	250	ASN
3	I	287	GLN
3	J	170	GLN
3	J	199	GLN
3	K	153	ASN
3	K	170	GLN
3	K	250	ASN
3	L	170	GLN
3	L	210	ASN
3	L	221	GLN
3	L	256	ASN
3	L	287	GLN
3	M	244	GLN
3	N	170	GLN
3	N	199	GLN
3	N	216	ASN
3	N	221	GLN
3	N	222	ASN
3	O	170	GLN
3	O	220	GLN
3	O	221	GLN

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Mol	Chain	Res	Type
3	O	250	ASN
3	O	287	GLN
3	O	291	ASN
3	P	170	GLN
3	P	199	GLN
3	P	210	ASN
3	P	221	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

### 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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	14/14 (100%)	0.02	0 100 100	36, 43, 52, 53	0
1	C	14/14 (100%)	-0.15	0 100 100	42, 48, 57, 58	0
1	E	14/14 (100%)	-0.08	0 100 100	33, 37, 49, 53	0
1	G	14/14 (100%)	-0.11	0 100 100	35, 41, 59, 59	0
2	B	14/14 (100%)	-0.14	0 100 100	34, 46, 58, 59	0
2	D	14/14 (100%)	-0.20	0 100 100	43, 50, 54, 55	0
2	F	14/14 (100%)	-0.07	0 100 100	33, 41, 45, 55	0
2	H	14/14 (100%)	-0.20	0 100 100	37, 44, 48, 52	0
3	I	150/151 (99%)	-0.06	0 100 100	34, 68, 103, 131	0
3	J	86/151 (56%)	0.09	3 (3%) 42 43	37, 60, 97, 105	0
3	K	150/151 (99%)	0.96	20 (13%) 4 3	51, 107, 137, 146	0
3	L	145/151 (96%)	0.36	9 (6%) 20 20	46, 68, 115, 142	0
3	M	150/151 (99%)	-0.01	3 (2%) 62 64	33, 58, 92, 123	0
3	N	85/151 (56%)	0.23	4 (4%) 30 31	38, 58, 92, 106	0
3	O	150/151 (99%)	0.39	14 (9%) 9 8	40, 79, 123, 136	0
3	P	82/151 (54%)	0.11	3 (3%) 39 41	43, 73, 103, 119	0
All	All	1110/1320 (84%)	0.24	56 (5%) 28 28	33, 67, 121, 146	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	K	175	THR	8.6
3	K	292	THR	8.4
3	K	174	ALA	6.4
3	K	282	PHE	5.0
3	K	273	TYR	4.8

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Mol	Chain	Res	Type	RSRZ
3	K	147	ILE	4.5
3	L	233	LYS	4.3
3	L	231	PRO	4.2
3	K	230	GLU	4.1
3	J	226	PHE	4.0
3	O	268	ALA	3.8
3	L	232	SER	3.8
3	K	231	PRO	3.7
3	K	264	ILE	3.5
3	K	177	GLY	3.5
3	O	175	THR	3.5
3	O	255	LYS	3.5
3	K	148	ARG	3.5
3	K	144	MSE	3.4
3	O	271	LEU	3.4
3	K	226	PHE	3.3
3	O	176	GLU	3.2
3	O	273	TYR	3.2
3	K	146	GLU	3.1
3	O	241	PHE	2.9
3	K	224	MSE	2.9
3	K	278	VAL	2.8
3	P	147	ILE	2.8
3	P	214	LEU	2.8
3	O	231	PRO	2.5
3	J	223	LEU	2.5
3	M	231	PRO	2.5
3	O	269	LYS	2.5
3	N	225	GLU	2.5
3	L	218	GLU	2.4
3	N	226	PHE	2.4
3	J	225	GLU	2.3
3	L	226	PHE	2.3
3	O	270	GLU	2.3
3	K	229	GLY	2.3
3	O	214	LEU	2.3
3	O	264	ILE	2.3
3	N	221	GLN	2.2
3	K	143	ASN	2.2
3	L	235	ARG	2.2
3	M	230	GLU	2.2
3	N	214	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
3	P	209	LEU	2.1
3	K	291	ASN	2.1
3	O	287	GLN	2.1
3	O	245	ALA	2.1
3	L	227	VAL	2.0
3	L	214	LEU	2.0
3	K	176	GLU	2.0
3	M	271	LEU	2.0
3	L	229	GLY	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.