Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:02 AM 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 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
http://wwpdb.org/validation/2016/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:

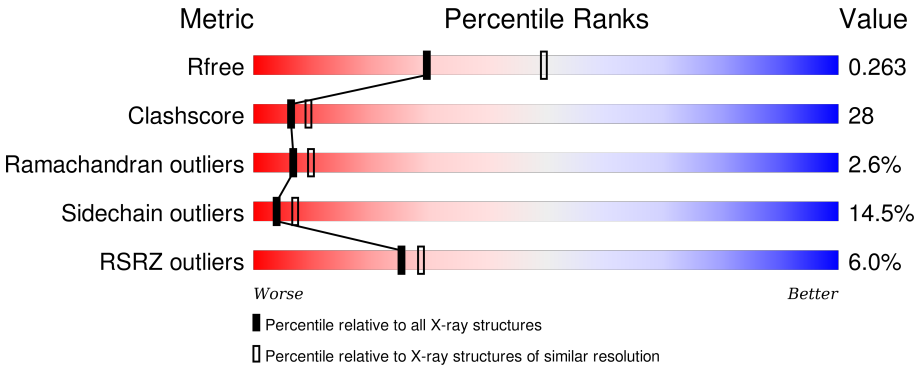
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.51 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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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 >=3, 2, 1 and 0 types of geometric quality criteria. 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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	14	21% 29% 50%
1	C	14	7% 50% 43%
1	E	14	36% 43% 21%
1	G	14	21% 36% 43%
2	B	14	7% 36% 57%

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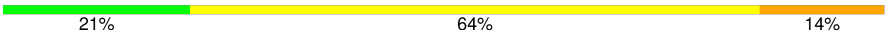
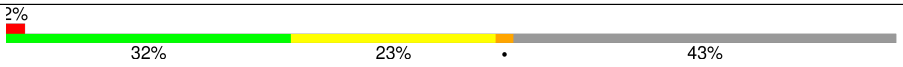
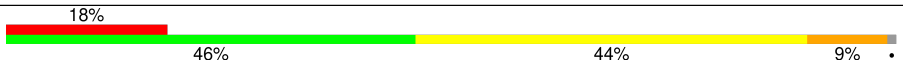
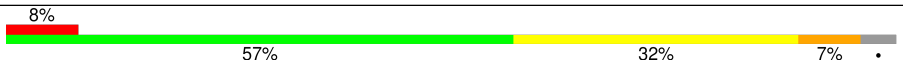
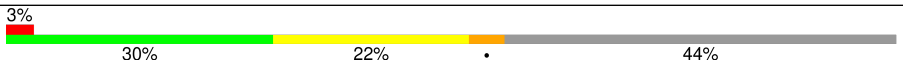
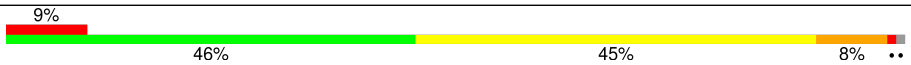
Mol	Chain	Length	Quality of chain
2	D	14	
2	F	14	
2	H	14	
3	I	151	
3	J	151	
3	K	151	
3	L	151	
3	M	151	
3	N	151	
3	O	151	
3	P	151	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10089 atoms, of which 0 are 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(*DAP*DGP*DCP*DAP*DTP*DAP*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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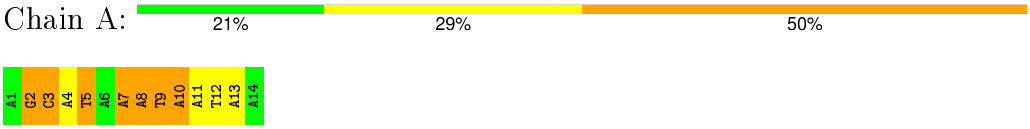
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	P	3	Total O 3 3	0	0

3 Residue-property plots (i)

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'

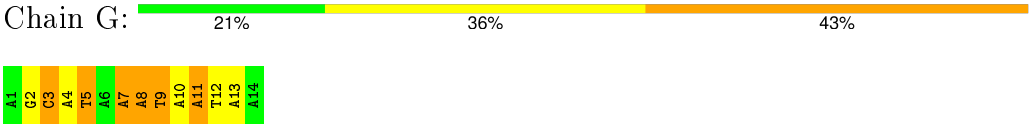
Chain C:

• 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*DC P*DT)-3'

Chain D:

• Molecule 2: 5'-D(*DTP*DTP*DAP*DTP*DTP*DAP*DTP*DTP*DTP*DAP*DTP*DGP*DC P*DT)-3'

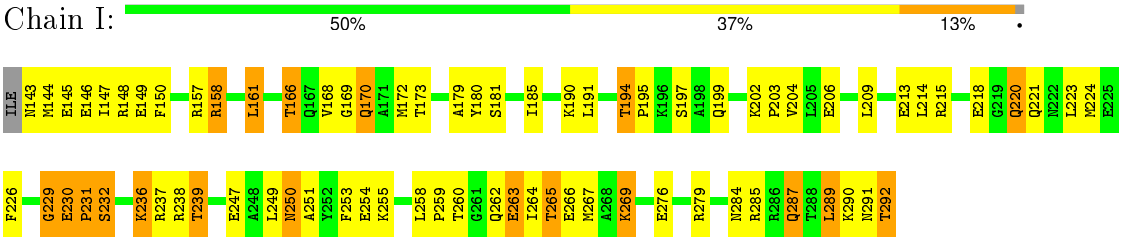
Chain F:

• Molecule 2: 5'-D(*DTP*DTP*DAP*DTP*DTP*DAP*DTP*DTP*DTP*DAP*DTP*DGP*DC P*DT)-3'

Chain H:

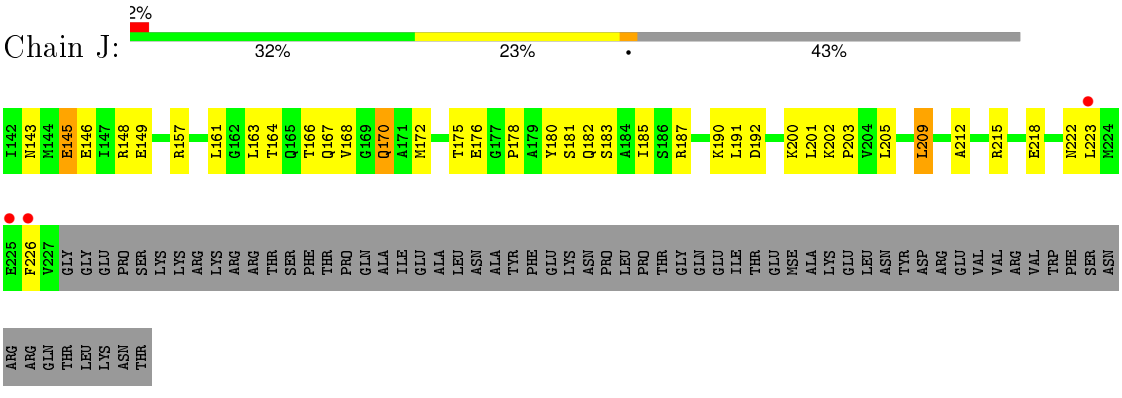
• Molecule 3: POU domain, class 6, transcription factor 1

Chain I:



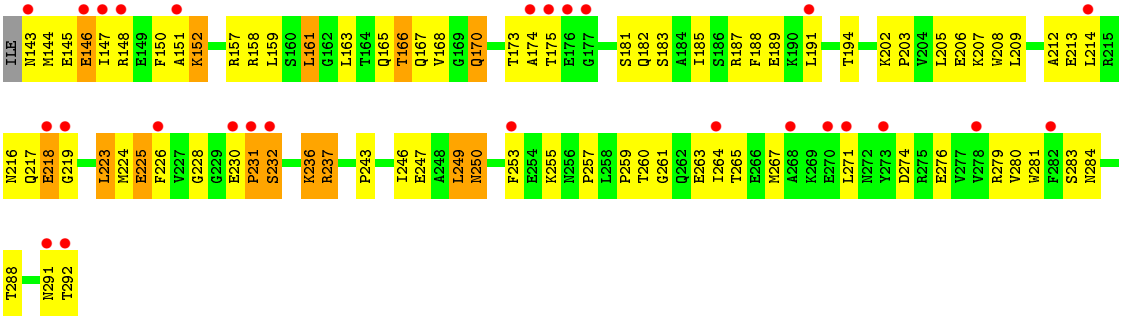
• Molecule 3: POU domain, class 6, transcription factor 1

Chain J:

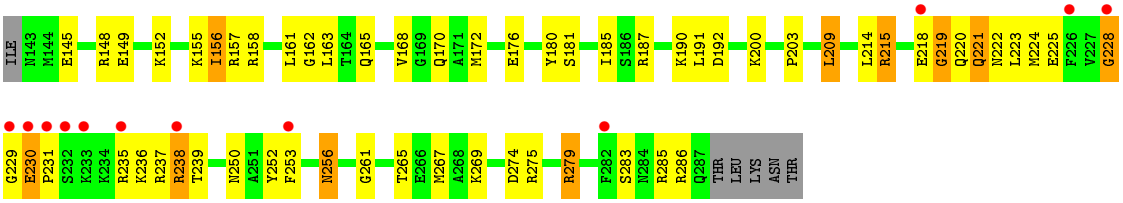


• Molecule 3: POU domain, class 6, transcription factor 1

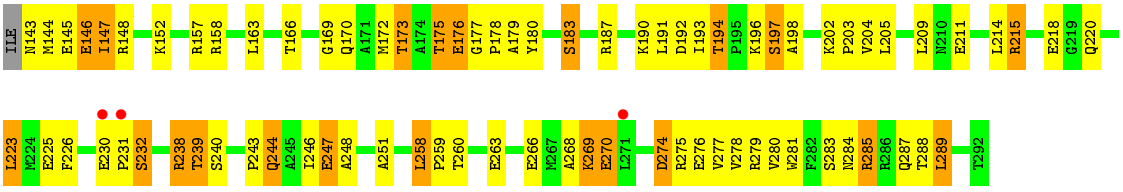
Chain K:



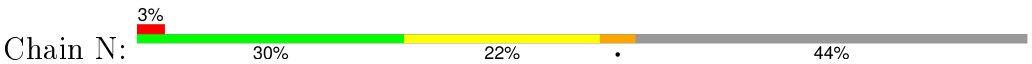
• Molecule 3: POU domain, class 6, transcription factor 1

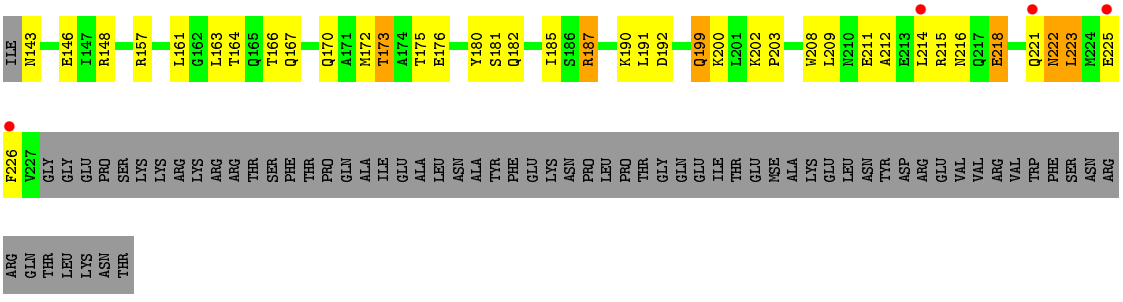


• Molecule 3: POU domain, class 6, transcription factor 1

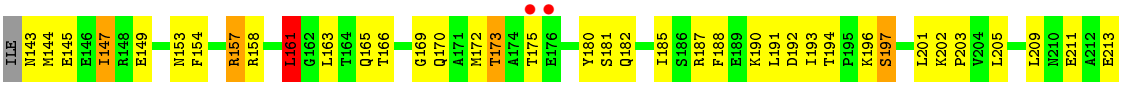


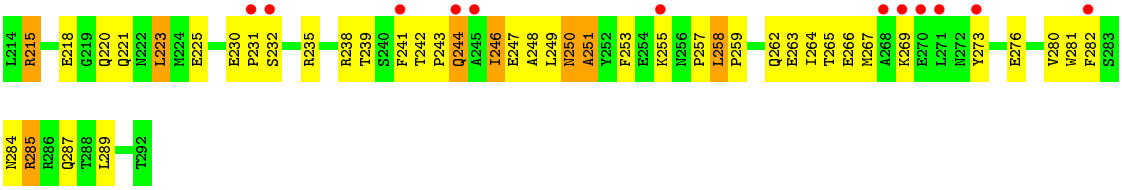
• Molecule 3: POU domain, class 6, transcription factor 1



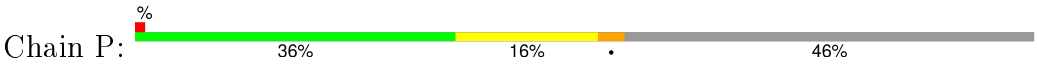


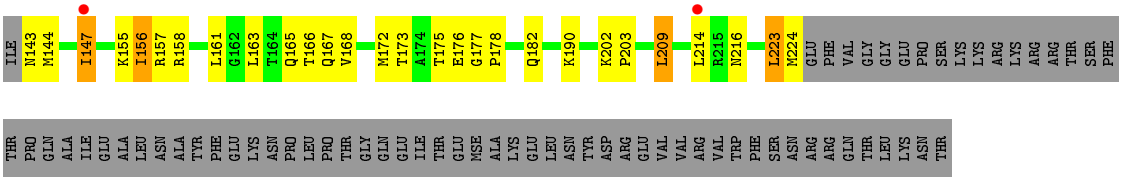
• Molecule 3: POU domain, class 6, transcription factor 1





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





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	65.06 (at 2.51Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.212 , 0.270 0.205 , 0.263	Depositor DCC
R_{free} test set	2672 reflections (5.11%)	DCC
Wilson B-factor (Å^2)	39.8	Xtriage
Anisotropy	0.886	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 76.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	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^2)	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.*

[1] Intensities estimated from amplitudes.

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

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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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
3	O	1166	0	1120	80	0
3	P	620	0	606	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

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 28.

All (512) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3: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	Interatomic distance (Å)	Clash overlap (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:157:ARG:CZ	3:L:209:LEU:HD13	2.18	0.73
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 (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
3	I	148/151 (98%)	123 (83%)	17 (12%)	8 (5%)	2 2
3	J	84/151 (56%)	78 (93%)	6 (7%)	0	100 100
3	K	148/151 (98%)	119 (80%)	22 (15%)	7 (5%)	3 3
3	L	143/151 (95%)	122 (85%)	16 (11%)	5 (4%)	4 6
3	M	148/151 (98%)	136 (92%)	10 (7%)	2 (1%)	14 24
3	N	83/151 (55%)	79 (95%)	3 (4%)	1 (1%)	16 29
3	O	148/151 (98%)	127 (86%)	19 (13%)	2 (1%)	14 24
3	P	80/151 (53%)	70 (88%)	9 (11%)	1 (1%)	15 26
All	All	982/1208 (81%)	854 (87%)	102 (10%)	26 (3%)	7 10

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

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Mol	Chain	Res	Type
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
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%)	2 4
3	J	69/129 (54%)	63 (91%)	6 (9%)	13 24
3	K	105/129 (81%)	89 (85%)	16 (15%)	3 6
3	L	115/129 (89%)	105 (91%)	10 (9%)	13 24
3	M	124/129 (96%)	96 (77%)	28 (23%)	1 1
3	N	68/129 (53%)	63 (93%)	5 (7%)	17 31
3	O	119/129 (92%)	98 (82%)	21 (18%)	2 4
3	P	62/129 (48%)	56 (90%)	6 (10%)	10 19
All	All	787/1032 (76%)	673 (86%)	114 (14%)	4 7

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 molecules 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^{th} 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^2)	Q<0.9
1	A	14/14 (100%)	0.10	0 100 100	36, 43, 52, 53	0
1	C	14/14 (100%)	-0.11	0 100 100	42, 48, 57, 58	0
1	E	14/14 (100%)	0.00	0 100 100	33, 37, 49, 53	0
1	G	14/14 (100%)	-0.05	0 100 100	35, 41, 59, 59	0
2	B	14/14 (100%)	-0.04	0 100 100	34, 46, 58, 59	0
2	D	14/14 (100%)	-0.13	0 100 100	43, 50, 54, 55	0
2	F	14/14 (100%)	0.02	0 100 100	33, 41, 45, 55	0
2	H	14/14 (100%)	-0.10	0 100 100	37, 44, 48, 52	0
3	I	146/151 (96%)	-0.02	0 100 100	34, 67, 102, 131	0
3	J	83/151 (54%)	0.18	3 (3%) 46 51	37, 60, 91, 103	0
3	K	146/151 (96%)	1.08	27 (18%) 2 2	51, 107, 136, 146	0
3	L	141/151 (93%)	0.49	12 (8%) 13 14	46, 67, 114, 142	0
3	M	146/151 (96%)	0.02	3 (2%) 67 71	33, 57, 91, 123	0
3	N	82/151 (54%)	0.27	4 (4%) 33 38	38, 58, 88, 106	0
3	O	146/151 (96%)	0.43	14 (9%) 10 11	40, 79, 122, 136	0
3	P	79/151 (52%)	0.14	2 (2%) 61 65	43, 73, 107, 119	0
All	All	1081/1320 (81%)	0.31	65 (6%) 25 28	33, 67, 121, 146	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	K	175	THR	8.9
3	K	292	THR	8.2
3	K	174	ALA	7.6
3	L	231	PRO	5.7
3	O	268	ALA	5.1

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Mol	Chain	Res	Type	RSRZ
3	K	231	PRO	4.8
3	L	232	SER	4.7
3	K	282	PHE	4.7
3	J	226	PHE	4.4
3	K	273	TYR	4.3
3	K	264	ILE	4.3
3	K	177	GLY	4.3
3	K	230	GLU	4.1
3	K	147	ILE	4.0
3	O	175	THR	3.9
3	L	233	LYS	3.7
3	J	223	LEU	3.7
3	L	229	GLY	3.6
3	O	271	LEU	3.6
3	L	218	GLU	3.5
3	K	226	PHE	3.4
3	K	148	ARG	3.2
3	O	176	GLU	3.1
3	O	245	ALA	3.1
3	K	146	GLU	3.1
3	O	273	TYR	3.0
3	O	255	LYS	3.0
3	P	214	LEU	3.0
3	K	218	GLU	2.9
3	K	214	LEU	2.8
3	K	291	ASN	2.7
3	K	176	GLU	2.7
3	L	282	PHE	2.7
3	K	151	ALA	2.6
3	O	270	GLU	2.6
3	O	231	PRO	2.6
3	N	225	GLU	2.6
3	K	278	VAL	2.6
3	J	225	GLU	2.6
3	P	147	ILE	2.5
3	L	253	PHE	2.5
3	L	226	PHE	2.5
3	O	241	PHE	2.5
3	K	143	ASN	2.4
3	L	230	GLU	2.4
3	M	231	PRO	2.4
3	O	244	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
3	L	238	ARG	2.3
3	K	270	GLU	2.3
3	N	226	PHE	2.3
3	L	235	ARG	2.2
3	K	271	LEU	2.2
3	K	232	SER	2.2
3	K	253	PHE	2.1
3	M	271	LEU	2.1
3	N	214	LEU	2.1
3	O	269	LYS	2.1
3	N	221	GLN	2.1
3	O	232	SER	2.1
3	L	228	GLY	2.1
3	K	219	GLY	2.0
3	K	191	LEU	2.0
3	O	282	PHE	2.0
3	K	268	ALA	2.0
3	M	230	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.