Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 06:01 am BST

PDB ID	:	6ERP
Title	:	Structure of the human mitochondrial transcription initiation complex at the LSP promoter
Authors	:	Hillen, H.S.; Morozov, Y.I.; Sarfallah, A.; Temiakov, D.; Cramer, P.
Deposited on	:	2017-10-18
Resolution	:	4.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

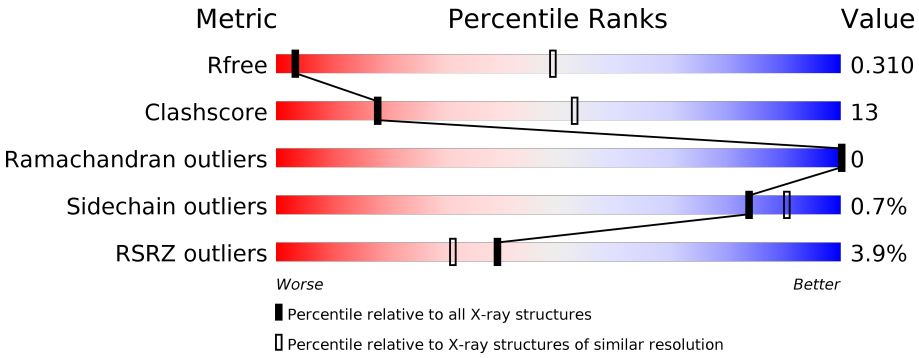
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 4.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1055 (5.20-3.80)
Clashscore	141614	1123 (5.20-3.80)
Ramachandran outliers	138981	1069 (5.20-3.80)
Sidechain outliers	138945	1050 (5.20-3.80)
RSRZ outliers	127900	1101 (5.30-3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	C	205	5% 67% 26% 6%
1	G	205	7% 71% 22% 6%
2	D	50	2% 26% 64% • 8%
2	H	50	2% 54% 38% 8%
3	E	50	2% 22% 64% • 10%
3	I	50	4% 26% 60% • 10%

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Mol	Chain	Length	Quality of chain
4	A	1128	4% 67% 22% 10%
4	B	1128	2% 68% 20% 11%
5	F	377	3% 58% 19% 24%
5	J	377	3% 59% 17% 24%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 27644 atoms, of which 42 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 protein called Transcription factor A, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	192	Total	C	N	O	S	0	0	0
			1615	1019	291	300	5			
1	G	192	Total	C	N	O	S	0	0	0
			1615	1019	291	300	5			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	41	ASN	-	expression tag	UNP Q00059
C	42	ALA	-	expression tag	UNP Q00059
C	49	SER	CYS	conflict	UNP Q00059
G	41	ASN	-	expression tag	UNP Q00059
G	42	ALA	-	expression tag	UNP Q00059
G	49	SER	CYS	conflict	UNP Q00059

- Molecule 2 is a DNA chain called Non-Template DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	46	Total	C	N	O	P	0	0	0
			952	454	176	277	45			
2	H	46	Total	C	N	O	P	0	0	0
			952	454	176	277	45			

- Molecule 3 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	45	Total	C	N	O	P	0	0	0
			907	434	163	266	44			
3	I	45	Total	C	N	O	P	0	0	0
			907	434	163	266	44			

- Molecule 4 is a protein called DNA-directed RNA polymerase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	1011	Total	C	N	O	S	0	0	0
			8028	5107	1452	1418	51			
4	B	1003	Total	C	N	O	S	0	0	0
			7974	5073	1444	1406	51			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	103	ASN	-	expression tag	UNP O00411
A	104	ALA	-	expression tag	UNP O00411
A	555	ALA	GLU	engineered mutation	UNP O00411
B	103	ASN	-	expression tag	UNP O00411
B	104	ALA	-	expression tag	UNP O00411
B	555	ALA	GLU	engineered mutation	UNP O00411

- Molecule 5 is a protein called Dimethyladenosine transferase 2, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
5	F	288	Total	C	H	N	O	S	0	0	0
			2347	1506	21	397	408	15			
5	J	288	Total	C	H	N	O	S	0	0	0
			2347	1506	21	397	408	15			

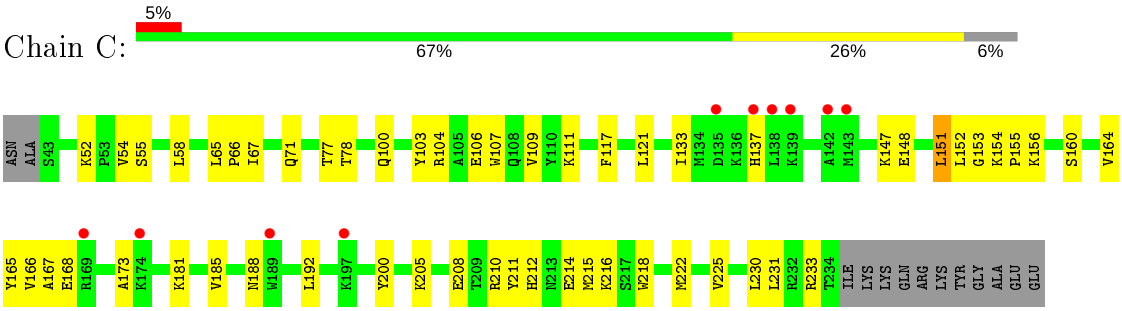
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	20	ASN	-	expression tag	UNP Q9H5Q4
F	21	ALA	GLY	conflict	UNP Q9H5Q4
J	20	ASN	-	expression tag	UNP Q9H5Q4
J	21	ALA	GLY	conflict	UNP Q9H5Q4

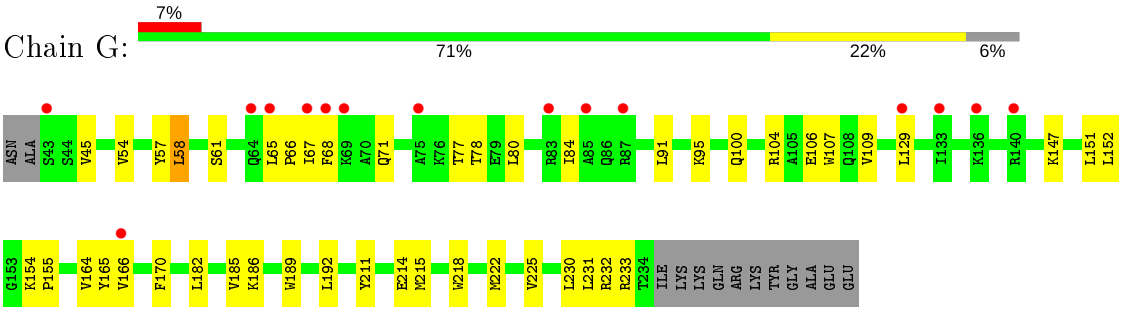
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

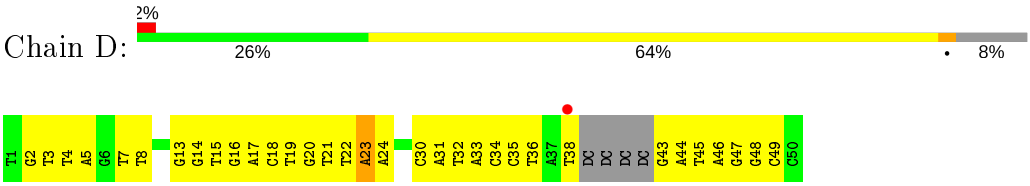
- Molecule 1: Transcription factor A, mitochondrial



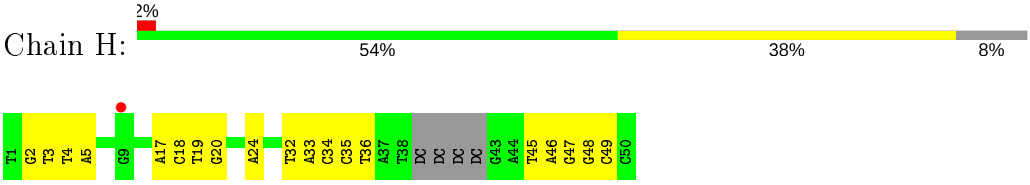
- Molecule 1: Transcription factor A, mitochondrial



- Molecule 2: Non-Template DNA

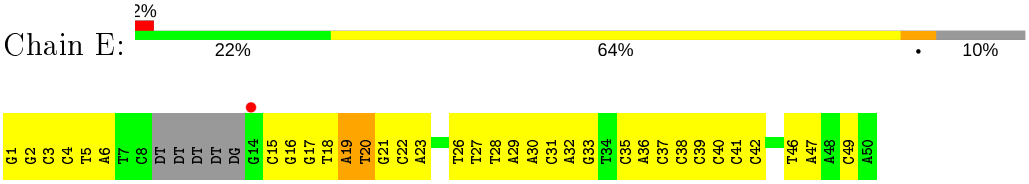


- Molecule 2: Non-Template DNA



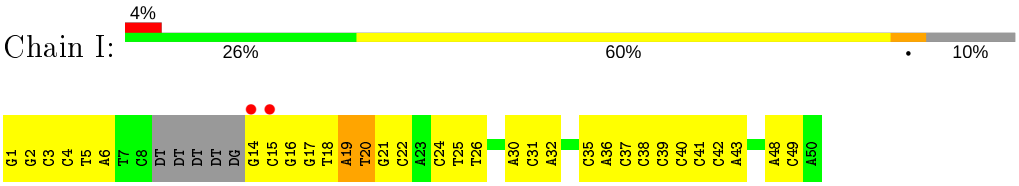
- Molecule 3: Template DNA

Chain E:



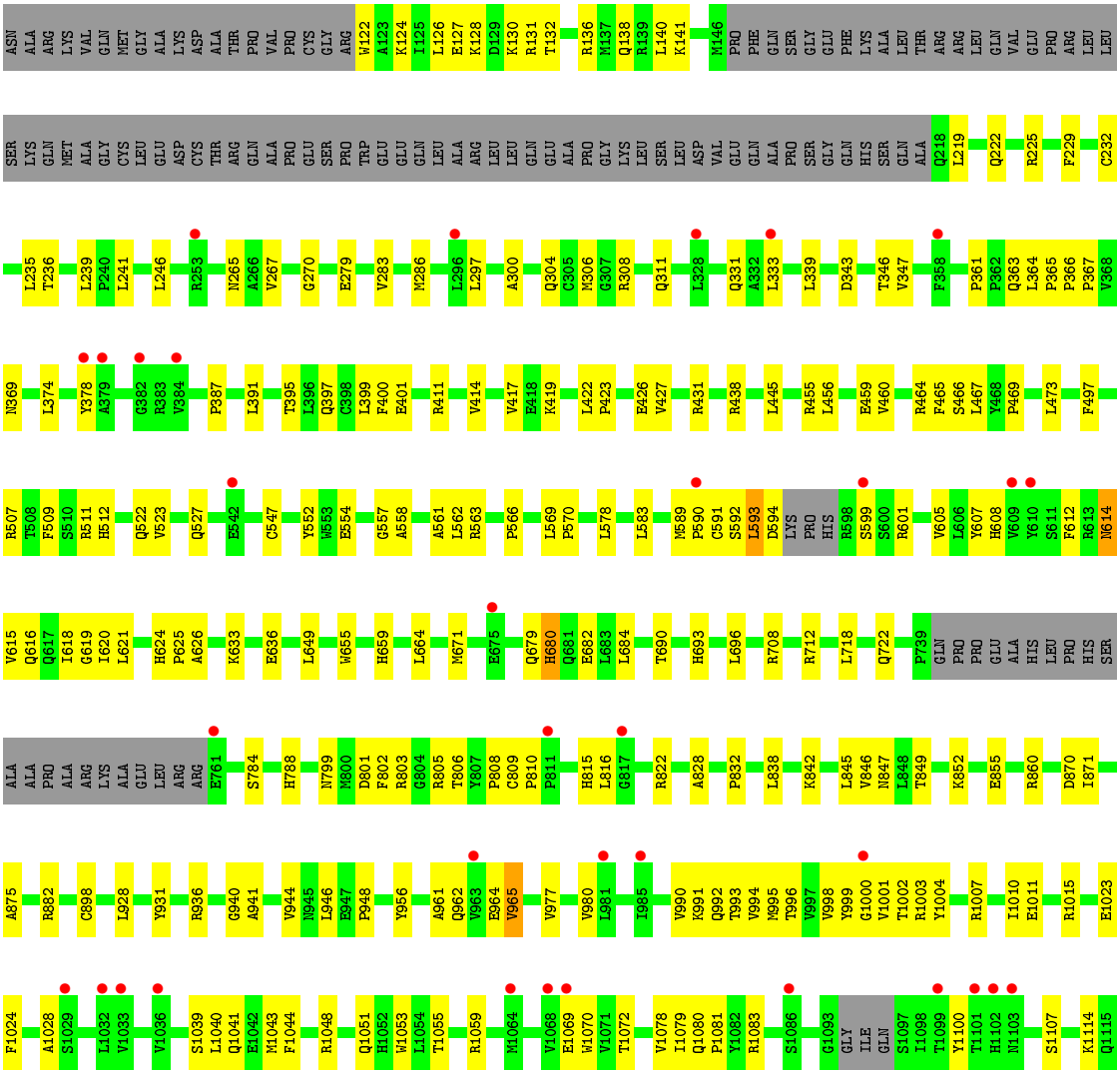
• Molecule 3: Template DNA

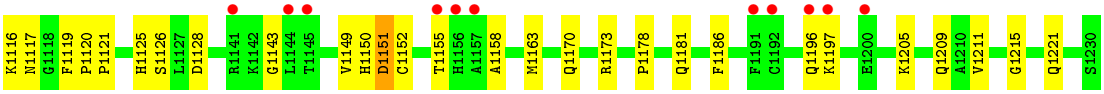
Chain I:



• Molecule 4: DNA-directed RNA polymerase, mitochondrial

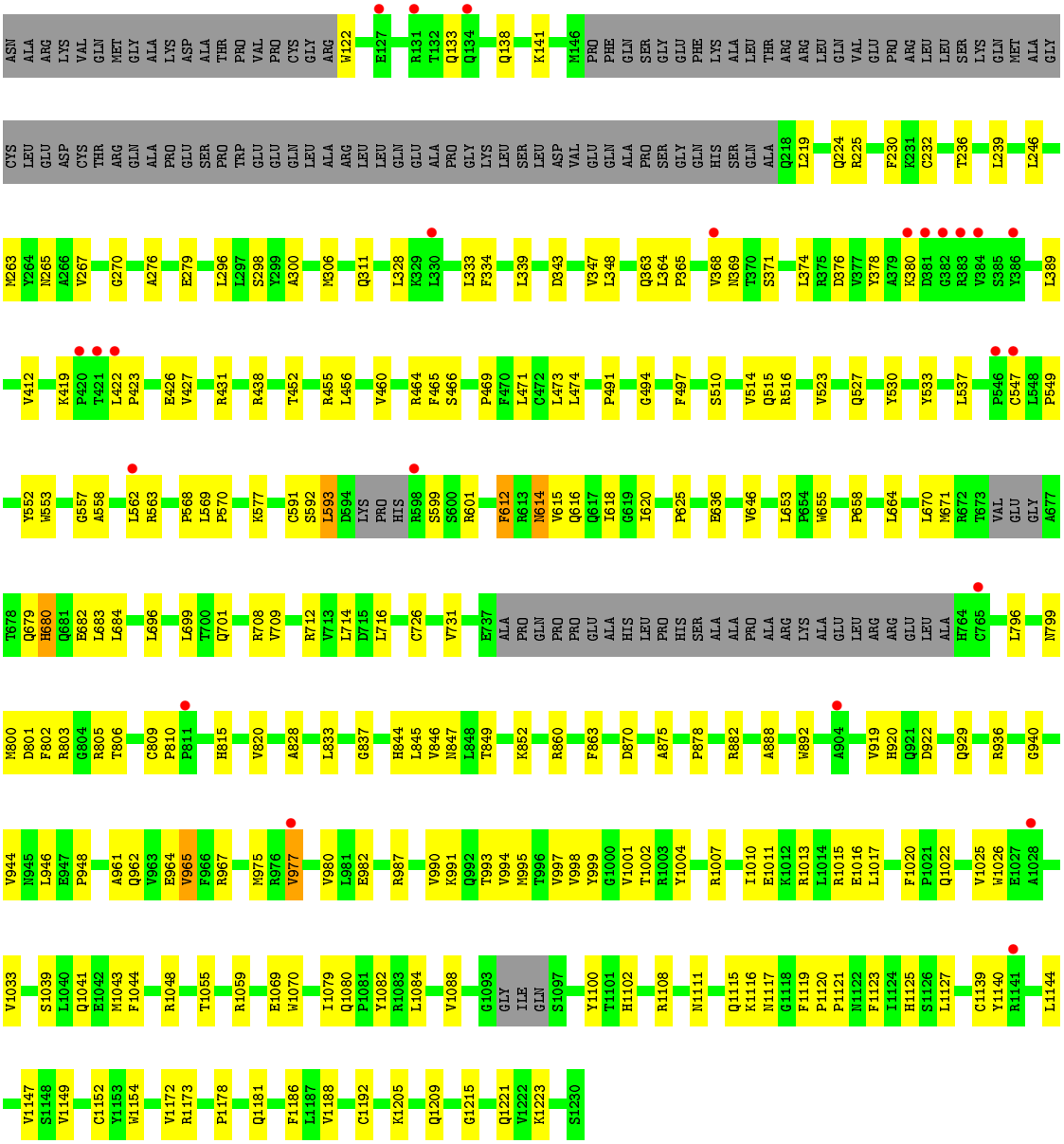
Chain A:





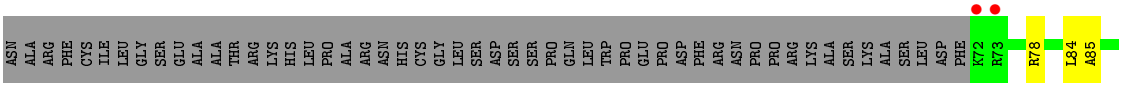
• Molecule 4: DNA-directed RNA polymerase, mitochondrial

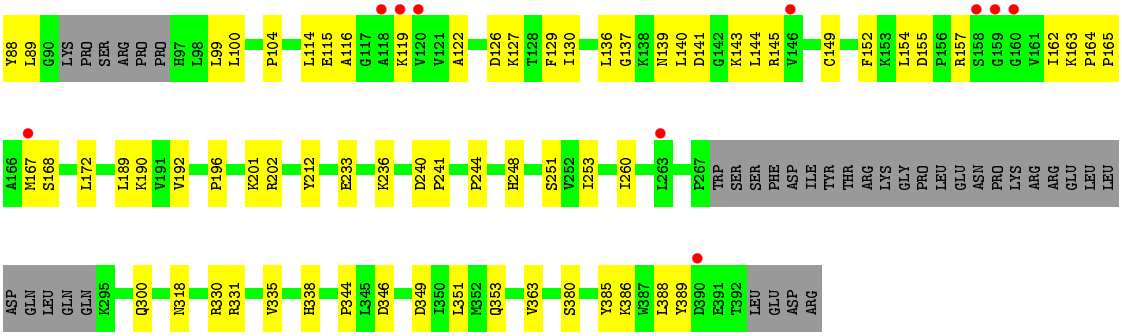
Chain B:



• Molecule 5: Dimethyladenosine transferase 2, mitochondrial

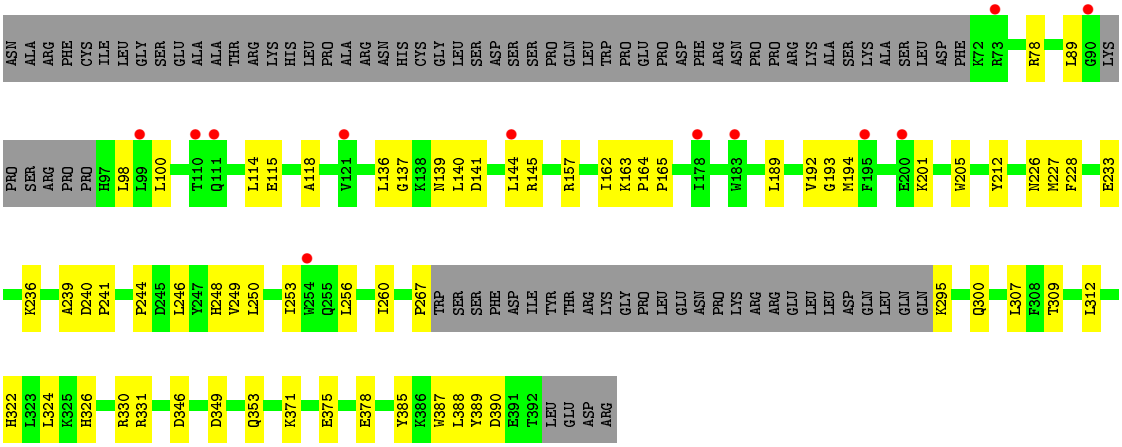
Chain F:





- Molecule 5: Dimethyladenosine transferase 2, mitochondrial

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	103.91Å 197.03Å 137.21Å 90.00° 99.87° 90.00°	Depositor
Resolution (Å)	49.58 – 4.50 49.58 – 4.50	Depositor EDS
% Data completeness (in resolution range)	98.7 (49.58-4.50) 98.8 (49.58-4.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.57 (at 4.45Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.270 , 0.310 0.270 , 0.310	Depositor DCC
R_{free} test set	1595 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	276.0	Xtriage
Anisotropy	0.256	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 290.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	27644	wwPDB-VP
Average B, all atoms (Å^2)	379.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	C	0.23	0/1646	0.35	0/2202
1	G	0.23	0/1646	0.36	0/2202
2	D	0.51	0/1068	0.95	1/1648 (0.1%)
2	H	0.53	0/1068	0.96	0/1648
3	E	0.57	0/1014	1.06	4/1557 (0.3%)
3	I	0.57	0/1014	1.05	4/1557 (0.3%)
4	A	0.23	0/8213	0.38	0/11132
4	B	0.23	0/8157	0.39	0/11053
5	F	0.24	0/2380	0.38	0/3213
5	J	0.23	0/2380	0.38	0/3213
All	All	0.30	0/28586	0.54	9/39425 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	20	DT	OP1-P-OP2	11.64	137.06	119.60
3	I	20	DT	OP1-P-OP2	11.11	136.27	119.60
3	E	19	DA	OP2-P-O3'	-10.97	81.06	105.20
3	I	19	DA	OP2-P-O3'	-10.76	81.54	105.20
3	E	19	DA	OP1-P-O3'	-9.04	85.32	105.20
3	I	19	DA	OP1-P-O3'	-8.87	85.70	105.20
3	I	19	DA	O4'-C1'-N9	6.64	112.65	108.00
3	E	19	DA	O4'-C1'-N9	6.19	112.33	108.00
2	D	23	DA	O4'-C1'-N9	5.01	111.51	108.00

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	C	1615	0	1655	55	0
1	G	1615	0	1655	46	0
2	D	952	0	523	36	0
2	H	952	0	523	19	0
3	E	907	0	508	63	0
3	I	907	0	508	52	0
4	A	8028	0	8092	209	0
4	B	7974	0	8039	198	0
5	F	2326	21	2375	63	0
5	J	2326	21	2375	51	0
All	All	27602	42	26253	725	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 13.

All (725) 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)
4:B:363:GLN:HB3	4:B:364:LEU:HG	1.28	1.13
4:A:363:GLN:HB3	4:A:364:LEU:HG	1.34	1.07
4:B:975:MET:HE2	4:B:977:VAL:HG23	1.31	1.04
1:G:152:LEU:HD21	1:G:230:LEU:HD13	1.41	1.02
5:F:89:LEU:HD11	5:F:116:ALA:HB1	1.42	1.00
5:J:114:LEU:HB3	5:J:140:LEU:HD11	1.43	0.99
5:F:114:LEU:HB3	5:F:140:LEU:HD11	1.45	0.98
4:B:1011:GLU:HG2	4:B:1025:VAL:HG22	1.46	0.98
3:I:19:DA:H2"	3:I:20:DT:H71	1.45	0.97
3:E:19:DA:H1'	3:E:20:DT:OP1	1.65	0.97
3:I:19:DA:H1'	3:I:20:DT:OP1	1.65	0.95
4:B:592:SER:HB2	4:B:599:SER:HB2	1.47	0.94
4:B:422:LEU:HG	4:B:427:VAL:HG21	1.56	0.88
4:B:422:LEU:HD21	4:B:427:VAL:HG11	1.56	0.88
4:B:592:SER:CB	4:B:599:SER:HB2	2.05	0.86
4:B:993:THR:HA	4:B:1010:ILE:HD11	1.56	0.86
1:G:147:LYS:O	1:G:151:LEU:HD13	1.79	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:37:DC:H2'	3:I:38:DC:C6	2.14	0.82
4:B:993:THR:HA	4:B:1010:ILE:CD1	2.11	0.81
1:C:231:LEU:O	1:C:233:ARG:NH1	2.14	0.81
3:I:19:DA:C2'	3:I:20:DT:H71	2.11	0.80
4:A:422:LEU:HD21	4:A:427:VAL:HG11	1.63	0.79
3:I:16:DG:H4'	4:B:618:ILE:HG22	1.62	0.79
1:G:152:LEU:CD2	1:G:230:LEU:HD13	2.11	0.79
4:B:999:TYR:O	4:B:1121:PRO:HB3	1.82	0.79
3:E:16:DG:H4'	4:A:618:ILE:HG22	1.63	0.79
3:E:37:DC:H2'	3:E:38:DC:C6	2.17	0.79
3:E:19:DA:H4'	3:E:20:DT:OP2	1.83	0.78
4:A:423:PRO:HG2	4:A:427:VAL:HG23	1.64	0.77
5:J:114:LEU:HD11	5:J:144:LEU:HD22	1.65	0.77
5:J:114:LEU:HB3	5:J:140:LEU:CD1	2.14	0.77
4:A:1178:PRO:HB2	4:A:1181:GLN:HB2	1.68	0.76
3:E:41:DC:H4'	3:E:42:DC:OP1	1.84	0.76
2:D:43:DG:H4'	2:D:44:DA:OP1	1.85	0.75
3:I:19:DA:H4'	3:I:20:DT:OP2	1.84	0.75
5:J:137:GLY:HA2	5:J:144:LEU:HD23	1.67	0.75
5:F:114:LEU:HB3	5:F:140:LEU:CD1	2.17	0.74
4:B:363:GLN:HB3	4:B:364:LEU:CG	2.14	0.74
3:I:41:DC:H4'	3:I:42:DC:OP1	1.87	0.74
2:H:20:DG:O6	3:I:32:DA:N6	2.21	0.74
3:I:36:DA:H2'	3:I:37:DC:C6	2.22	0.74
1:G:107:TRP:CH2	2:H:24:DA:H5"	2.23	0.74
3:I:36:DA:H2'	3:I:37:DC:H6	1.53	0.74
4:A:655:TRP:HB3	4:A:696:LEU:HD22	1.69	0.74
4:B:712:ARG:NH2	4:B:875:ALA:O	2.21	0.74
4:A:246:LEU:HD22	4:A:267:VAL:HG21	1.69	0.73
5:J:137:GLY:CA	5:J:144:LEU:HD23	2.18	0.73
4:B:363:GLN:CB	4:B:364:LEU:HG	2.15	0.73
4:A:239:LEU:HD11	4:A:270:GLY:HA3	1.72	0.72
1:C:78:THR:HG23	2:D:19:DT:H4'	1.71	0.72
1:C:148:GLU:O	1:C:152:LEU:HD13	1.89	0.72
4:B:1015:ARG:CZ	4:B:1025:VAL:HG11	2.19	0.72
4:B:423:PRO:HG2	4:B:427:VAL:HG23	1.72	0.72
5:F:137:GLY:HA2	5:F:144:LEU:HD23	1.71	0.72
4:A:1072:THR:HG22	4:A:1126:SER:HB2	1.72	0.71
4:B:422:LEU:CG	4:B:427:VAL:HG21	2.20	0.71
1:C:168:GLU:HB2	4:A:122:TRP:CZ2	2.26	0.71
1:G:214:GLU:OE2	4:B:133:GLN:NE2	2.24	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:137:GLY:CA	5:F:144:LEU:HD23	2.21	0.71
4:B:944:VAL:HG23	4:B:946:LEU:HD13	1.70	0.70
4:A:936:ARG:HB2	4:A:1215:GLY:H	1.56	0.70
2:H:4:DT:H2'	2:H:5:DA:C8	2.25	0.70
4:A:363:GLN:HB3	4:A:364:LEU:CG	2.19	0.70
4:B:726:CYS:H	4:B:731:VAL:HB	1.57	0.70
5:J:100:LEU:HD13	5:J:189:LEU:HD11	1.74	0.70
5:F:349:ASP:O	5:F:353:GLN:HG2	1.92	0.70
4:B:809:CYS:HB2	4:B:810:PRO:HD3	1.73	0.70
5:F:144:LEU:HD12	5:F:145:ARG:N	2.07	0.69
4:B:975:MET:HE2	4:B:977:VAL:CG2	2.15	0.69
5:J:100:LEU:HD22	5:J:189:LEU:HD21	1.73	0.69
5:F:236:LYS:O	5:F:251:SER:OG	2.11	0.69
4:A:809:CYS:HB2	4:A:810:PRO:HD3	1.75	0.69
3:I:16:DG:H5"	4:B:618:ILE:HG22	1.75	0.69
3:I:18:DT:H5"	5:J:330:ARG:HG2	1.74	0.69
5:J:144:LEU:HD12	5:J:145:ARG:N	2.07	0.69
4:A:944:VAL:HG23	4:A:946:LEU:HD13	1.73	0.69
3:I:16:DG:C5'	4:B:618:ILE:HG22	2.22	0.69
5:J:137:GLY:O	5:J:141:ASP:N	2.14	0.69
3:E:36:DA:H2'	3:E:37:DC:C6	2.29	0.68
5:J:349:ASP:O	5:J:353:GLN:HG2	1.94	0.68
4:A:363:GLN:CB	4:A:364:LEU:HG	2.19	0.68
5:F:89:LEU:CD1	5:F:116:ALA:HB1	2.22	0.68
4:A:1120:PRO:HB2	4:A:1121:PRO:HD3	1.74	0.68
3:I:17:DG:OP2	4:B:1100:TYR:HA	1.94	0.68
3:E:16:DG:C5	4:A:616:GLN:HG2	2.29	0.68
4:B:422:LEU:CD1	4:B:427:VAL:HG21	2.24	0.67
4:B:219:LEU:HD23	4:B:219:LEU:H	1.60	0.67
5:F:84:LEU:HB3	5:F:88:TYR:HE2	1.58	0.67
4:B:671:MET:SD	4:B:684:LEU:HD11	2.34	0.67
2:D:34:DC:H2"	2:D:35:DC:C6	2.30	0.67
3:E:35:DC:H2"	3:E:36:DA:C8	2.29	0.67
5:F:100:LEU:HD13	5:F:189:LEU:HD11	1.76	0.66
5:F:100:LEU:HD22	5:F:189:LEU:HD21	1.76	0.66
4:B:1004:TYR:HB2	4:B:1007:ARG:HB2	1.77	0.66
4:B:1015:ARG:HA	4:B:1022:GLN:OE1	1.96	0.66
4:A:607:TYR:CZ	5:F:388:LEU:HD13	2.30	0.66
1:G:54:VAL:HG12	1:G:58:LEU:HB3	1.77	0.66
4:A:219:LEU:HD23	4:A:219:LEU:H	1.60	0.66
3:I:37:DC:H2'	3:I:38:DC:C5	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:89:LEU:HD11	5:F:116:ALA:CB	2.21	0.66
4:A:363:GLN:HA	4:A:365:PRO:HD3	1.78	0.65
3:E:19:DA:C1'	3:E:20:DT:OP1	2.44	0.65
4:A:936:ARG:HB2	4:A:1215:GLY:N	2.12	0.65
4:A:815:HIS:HD2	4:A:1149:VAL:HG22	1.61	0.65
4:A:236:THR:HG23	4:A:473:LEU:HD23	1.79	0.64
4:A:1043:MET:HG3	4:A:1044:PHE:CD2	2.32	0.64
4:A:591:CYS:O	4:A:593:LEU:HD23	1.97	0.64
5:F:114:LEU:HD11	5:F:144:LEU:HD22	1.78	0.64
5:F:144:LEU:HD12	5:F:145:ARG:H	1.62	0.64
4:A:422:LEU:HG	4:A:427:VAL:HG21	1.78	0.64
4:B:699:LEU:HD11	4:B:800:MET:HG3	1.79	0.64
3:I:16:DG:H2'	3:I:16:DG:OP1	1.98	0.63
3:I:16:DG:C4'	4:B:618:ILE:HG22	2.29	0.63
4:B:625:PRO:HB2	5:J:385:TYR:CZ	2.34	0.63
3:E:1:DG:H2"	3:E:2:DG:C8	2.33	0.63
1:C:165:TYR:CE1	1:C:192:LEU:HD11	2.33	0.63
4:A:1004:TYR:HB2	4:A:1007:ARG:HB2	1.79	0.63
2:H:4:DT:H2"	2:H:5:DA:O5'	1.97	0.63
5:J:144:LEU:HD12	5:J:145:ARG:H	1.64	0.63
2:H:4:DT:H4'	2:H:5:DA:OP1	1.99	0.63
4:A:391:LEU:HD22	4:A:395:THR:HG21	1.80	0.62
3:E:16:DG:H5"	4:A:618:ILE:HG22	1.81	0.62
3:E:5:DT:H2"	3:E:6:DA:C8	2.34	0.62
4:B:1069:GLU:HG2	4:B:1079:ILE:HG23	1.81	0.62
2:D:14:DG:H2'	2:D:15:DT:H71	1.81	0.62
3:I:15:DC:H2"	3:I:16:DG:OP1	1.99	0.62
5:J:89:LEU:HD21	5:J:118:ALA:HB2	1.81	0.62
4:A:940:GLY:O	4:A:944:VAL:HG22	2.00	0.62
4:A:1149:VAL:HG12	4:A:1150:HIS:ND1	2.14	0.62
4:B:655:TRP:HB3	4:B:696:LEU:HD22	1.81	0.61
5:J:240:ASP:HB2	5:J:241:PRO:HD2	1.81	0.61
4:B:1001:VAL:O	4:B:1002:THR:OG1	2.11	0.61
5:J:322:HIS:HB3	5:J:389:TYR:CZ	2.34	0.61
4:B:1120:PRO:HB2	4:B:1121:PRO:HD3	1.81	0.61
4:A:456:LEU:O	4:A:460:VAL:HG23	2.00	0.61
3:E:17:DG:C2'	3:E:18:DT:H71	2.30	0.61
4:A:1069:GLU:HG2	4:A:1079:ILE:HG23	1.81	0.61
2:D:45:DT:H2"	2:D:46:DA:C8	2.36	0.61
4:A:1001:VAL:O	4:A:1002:THR:OG1	2.08	0.60
4:B:438:ARG:NH1	4:B:636:GLU:OE2	2.27	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:849:THR:HA	4:B:888:ALA:HB1	1.83	0.60
5:J:378:GLU:OE2	5:J:387:TRP:NE1	2.33	0.60
4:A:369:ASN:ND2	4:A:690:THR:O	2.34	0.60
4:A:1070:TRP:HA	4:A:1186:PHE:CE1	2.36	0.60
4:A:1055:THR:O	4:A:1059:ARG:HG3	2.02	0.60
2:D:4:DT:H4'	2:D:5:DA:OP1	2.01	0.60
5:F:240:ASP:HB2	5:F:241:PRO:HD2	1.81	0.60
3:I:19:DA:C1'	3:I:20:DT:OP1	2.45	0.60
4:A:423:PRO:CG	4:A:427:VAL:HG23	2.31	0.60
4:B:423:PRO:CG	4:B:426:GLU:HB3	2.32	0.60
1:G:186:LYS:HE2	3:I:43:DA:H4'	1.83	0.60
4:A:803:ARG:HD3	4:A:1125:HIS:CD2	2.36	0.60
4:B:1070:TRP:HA	4:B:1186:PHE:CE1	2.37	0.60
2:D:4:DT:H2"	2:D:5:DA:O5'	2.01	0.60
4:B:671:MET:SD	4:B:680:HIS:ND1	2.75	0.60
3:E:37:DC:H2'	3:E:38:DC:C5	2.37	0.60
5:J:236:LYS:HG2	5:J:246:LEU:HD22	1.83	0.60
4:B:1011:GLU:OE2	4:B:1026:TRP:HA	2.01	0.59
3:E:16:DG:C4	4:A:616:GLN:HB3	2.37	0.59
4:A:522:GLN:OE1	4:A:561:ALA:HB1	2.02	0.59
4:A:1039:SER:O	4:A:1043:MET:HG2	2.03	0.59
4:B:423:PRO:CG	4:B:427:VAL:HG23	2.32	0.59
4:A:283:VAL:HA	4:A:286:MET:CE	2.32	0.59
4:B:683:LEU:HD12	4:B:1079:ILE:HG12	1.83	0.59
3:E:36:DA:H2'	3:E:37:DC:H6	1.67	0.59
4:B:708:ARG:HD3	4:B:828:ALA:HA	1.85	0.58
4:B:940:GLY:O	4:B:944:VAL:HG22	2.02	0.58
4:B:977:VAL:HA	4:B:980:VAL:HG22	1.84	0.58
4:B:419:LYS:HE3	4:B:431:ARG:HH22	1.67	0.58
2:D:4:DT:H2'	2:D:5:DA:C8	2.38	0.58
3:E:41:DC:H2'	3:E:42:DC:C6	2.37	0.58
1:G:65:LEU:HD11	1:G:77:THR:HG23	1.84	0.58
4:A:847:ASN:OD1	4:A:860:ARG:NH1	2.36	0.58
3:I:18:DT:H2"	3:I:19:DA:H8	1.68	0.58
4:A:1041:GLN:HB3	4:A:1048:ARG:HD2	1.85	0.58
5:J:309:THR:OG1	5:J:375:GLU:OE2	2.07	0.58
4:B:1055:THR:O	4:B:1059:ARG:HG3	2.04	0.58
3:E:20:DT:H2"	3:E:21:DG:C8	2.39	0.58
3:I:35:DC:H2"	3:I:36:DA:C8	2.39	0.58
4:B:423:PRO:HD2	4:B:427:VAL:HG23	1.86	0.58
1:C:211:TYR:O	1:C:215:MET:HG2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:152:LEU:HD21	1:G:230:LEU:CD1	2.27	0.58
4:B:1178:PRO:HB2	4:B:1181:GLN:HB2	1.85	0.57
1:C:155:PRO:CG	1:C:214:GLU:HB3	2.34	0.57
4:B:1043:MET:HG3	4:B:1044:PHE:CD2	2.39	0.57
1:C:133:ILE:HG23	1:C:137:HIS:HE1	1.68	0.57
5:F:318:ASN:HD22	5:F:389:TYR:HE2	1.51	0.57
4:A:708:ARG:HD3	4:A:828:ALA:HA	1.85	0.57
4:B:683:LEU:CD1	4:B:1079:ILE:HG12	2.35	0.57
1:C:155:PRO:HG3	1:C:214:GLU:HB3	1.86	0.57
5:F:84:LEU:HB3	5:F:88:TYR:CE2	2.39	0.57
3:I:16:DG:C4	4:B:616:GLN:HB3	2.39	0.57
4:B:1017:LEU:O	4:B:1020:PHE:N	2.35	0.57
1:C:67:ILE:O	1:C:71:GLN:HG2	2.04	0.57
4:B:940:GLY:HA2	4:B:1044:PHE:HE1	1.70	0.57
1:G:67:ILE:O	1:G:71:GLN:HG2	2.05	0.57
4:A:509:PHE:CE1	4:A:566:PRO:HA	2.40	0.57
4:A:996:THR:O	4:A:1000:GLY:N	2.35	0.57
4:B:997:VAL:HG13	4:B:1001:VAL:CG2	2.33	0.57
4:A:232:CYS:SG	4:A:473:LEU:HD11	2.45	0.56
4:B:614:ASN:OD1	4:B:614:ASN:N	2.38	0.56
4:A:306:MET:HG2	4:A:311:GLN:HG3	1.87	0.56
4:B:1011:GLU:CG	4:B:1025:VAL:HG22	2.29	0.56
4:B:680:HIS:NE2	4:B:802:PHE:HB2	2.20	0.56
5:F:155:ASP:OD1	5:F:168:SER:HA	2.06	0.56
4:A:815:HIS:CD2	4:A:1149:VAL:HG22	2.39	0.56
4:A:962:GLN:O	4:A:965:VAL:HG22	2.05	0.56
3:E:41:DC:H2"	3:E:42:DC:O5'	2.05	0.56
1:C:168:GLU:HB2	4:A:122:TRP:HZ2	1.70	0.56
4:B:363:GLN:HA	4:B:365:PRO:HD3	1.86	0.56
3:E:19:DA:N9	3:E:20:DT:H72	2.20	0.56
5:J:164:PRO:HG2	5:J:165:PRO:HD3	1.88	0.56
4:A:614:ASN:OD1	4:A:614:ASN:N	2.39	0.55
3:E:16:DG:C4'	4:A:618:ILE:HG22	2.35	0.55
2:H:34:DC:H2"	2:H:35:DC:C6	2.41	0.55
3:I:38:DC:C2	3:I:39:DC:C5	2.94	0.55
4:B:592:SER:OG	4:B:599:SER:HB2	2.05	0.55
4:B:994:VAL:HG12	4:B:998:VAL:CG2	2.36	0.55
4:B:833:LEU:HB3	4:B:837:GLY:HA3	1.89	0.55
4:B:423:PRO:HD2	4:B:427:VAL:CG2	2.37	0.55
4:B:803:ARG:HD3	4:B:1125:HIS:CD2	2.42	0.55
2:D:47:DG:H2"	2:D:48:DG:C8	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:164:PRO:HG2	5:F:165:PRO:HD3	1.88	0.55
5:J:240:ASP:HB2	5:J:241:PRO:CD	2.36	0.55
4:A:414:VAL:HG13	4:A:788:HIS:HB2	1.88	0.55
4:A:956:TYR:CD1	4:A:991:LYS:HA	2.42	0.55
4:B:997:VAL:HG13	4:B:1001:VAL:HG22	1.88	0.55
4:B:1039:SER:O	4:B:1043:MET:HG2	2.06	0.55
4:A:832:PRO:O	4:A:1158:ALA:HB2	2.06	0.55
2:D:36:DT:O2	4:A:615:VAL:HG11	2.06	0.55
4:B:422:LEU:HG	4:B:427:VAL:CG2	2.34	0.55
3:E:38:DC:C2	3:E:39:DC:C5	2.95	0.55
1:C:167:ALA:HB3	4:A:122:TRP:HH2	1.72	0.54
2:D:46:DA:H2"	2:D:47:DG:C8	2.42	0.54
5:F:240:ASP:HB2	5:F:241:PRO:CD	2.37	0.54
1:G:154:LYS:CG	1:G:155:PRO:HD2	2.38	0.54
3:I:1:DG:H2"	3:I:2:DG:C8	2.42	0.54
1:G:58:LEU:HD22	3:I:30:DA:N3	2.23	0.54
4:B:1139:CYS:HB3	4:B:1144:LEU:HB2	1.89	0.54
4:B:796:LEU:HD22	4:B:810:PRO:HG2	1.89	0.54
1:G:182:LEU:HD23	3:I:42:DC:C2	2.42	0.54
4:A:607:TYR:CE1	5:F:388:LEU:HD13	2.43	0.54
3:I:5:DT:H2"	3:I:6:DA:C8	2.43	0.54
3:E:16:DG:H5"	4:A:618:ILE:CG2	2.37	0.54
4:A:846:VAL:HG21	4:A:860:ARG:O	2.07	0.54
4:B:562:LEU:HD23	4:B:563:ARG:N	2.22	0.54
1:G:57:TYR:OH	2:H:20:DG:H1'	2.07	0.54
4:B:1041:GLN:HB3	4:B:1048:ARG:HD2	1.90	0.54
1:C:58:LEU:HD22	3:E:30:DA:N3	2.22	0.54
4:A:422:LEU:CD1	4:A:427:VAL:HG21	2.38	0.54
4:B:376:ASP:OD2	4:B:1173:ARG:NH1	2.40	0.54
1:C:154:LYS:HE2	1:C:215:MET:SD	2.48	0.54
5:F:126:ASP:HB3	5:F:129:PHE:HD2	1.72	0.54
5:F:201:LYS:HE3	5:F:233:GLU:OE2	2.08	0.54
4:A:400:PHE:CE1	4:A:664:LEU:HD13	2.43	0.54
4:B:1004:TYR:HB3	4:B:1007:ARG:HD2	1.90	0.54
4:A:679:GLN:O	4:A:682:GLU:HG2	2.08	0.54
4:A:852:LYS:HB3	4:A:855:GLU:HB2	1.89	0.54
4:B:306:MET:HG2	4:B:311:GLN:HG3	1.90	0.54
4:B:1119:PHE:HB3	4:B:1120:PRO:HD3	1.90	0.53
4:B:592:SER:O	4:B:593:LEU:HG	2.08	0.53
2:H:3:DT:C6	2:H:4:DT:H72	2.43	0.53
4:A:593:LEU:HB3	4:A:626:ALA:HB1	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1015:ARG:HG2	4:B:1022:GLN:HG3	1.90	0.53
2:D:38:DT:H72	5:F:202:ARG:NE	2.23	0.53
3:E:41:DC:H2"	3:E:42:DC:C5'	2.39	0.53
1:G:78:THR:HG23	2:H:19:DT:O4'	2.08	0.53
3:E:16:DG:C5'	4:A:618:ILE:HG22	2.38	0.53
4:A:940:GLY:HA2	4:A:1044:PHE:CE1	2.43	0.53
2:H:36:DT:O2	4:B:615:VAL:HG11	2.09	0.53
1:G:154:LYS:HG2	1:G:155:PRO:HD2	1.90	0.53
4:A:138:GLN:HA	4:A:141:LYS:HE2	1.90	0.53
4:A:464:ARG:NH1	4:A:465:PHE:H	2.07	0.53
4:A:1002:THR:H	4:A:1007:ARG:NH2	2.06	0.53
4:B:997:VAL:CG2	4:B:1033:VAL:HG13	2.39	0.53
1:C:54:VAL:HG12	1:C:58:LEU:HB3	1.91	0.53
1:C:78:THR:HG23	2:D:19:DT:C4'	2.39	0.53
4:A:562:LEU:HD23	4:A:563:ARG:N	2.23	0.53
4:B:655:TRP:O	4:B:696:LEU:HB3	2.09	0.53
5:F:152:PHE:CZ	5:F:196:PRO:HD3	2.44	0.53
4:A:1116:LYS:HG3	4:A:1117:ASN:N	2.24	0.53
1:G:164:VAL:HG13	4:B:122:TRP:CH2	2.44	0.53
2:H:2:DG:C8	2:H:3:DT:H72	2.43	0.53
4:B:1088:VAL:O	4:B:1102:HIS:N	2.42	0.53
1:C:155:PRO:HB3	1:C:210:ARG:NH1	2.24	0.53
4:B:701:GLN:NE2	4:B:1140:TYR:HB2	2.24	0.52
3:E:17:DG:H2"	3:E:18:DT:H71	1.91	0.52
5:J:236:LYS:HA	5:J:246:LEU:HB3	1.91	0.52
5:J:322:HIS:HB3	5:J:389:TYR:CE2	2.44	0.52
4:A:1120:PRO:CB	4:A:1121:PRO:HD3	2.39	0.52
4:A:607:TYR:HE2	4:A:624:HIS:HA	1.75	0.52
5:F:344:PRO:HG3	5:F:385:TYR:CE2	2.44	0.52
1:G:211:TYR:O	1:G:215:MET:HG2	2.09	0.52
4:A:928:LEU:HG	4:A:998:VAL:HG21	1.91	0.52
1:C:154:LYS:HD2	1:C:218:TRP:CZ3	2.44	0.52
3:I:20:DT:H2"	3:I:21:DG:C8	2.45	0.52
3:E:26:DT:C6	3:E:27:DT:H72	2.44	0.52
1:G:154:LYS:HE3	1:G:218:TRP:CE3	2.45	0.52
4:A:718:LEU:HB3	4:A:722:GLN:HE21	1.75	0.52
4:B:618:ILE:HD12	4:B:618:ILE:O	2.10	0.52
2:D:14:DG:C2'	2:D:15:DT:H71	2.39	0.52
3:E:2:DG:H2"	3:E:3:DC:C6	2.45	0.52
4:A:594:ASP:OD2	4:A:633:LYS:NZ	2.37	0.52
3:E:20:DT:H2"	3:E:21:DG:H8	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1080:GLN:NE2	4:B:1115:GLN:OE1	2.41	0.52
5:F:244:PRO:O	5:F:331:ARG:NH2	2.42	0.52
4:A:1150:HIS:NE2	4:A:1152:CYS:SG	2.81	0.52
1:C:107:TRP:CH2	2:D:24:DA:H4'	2.45	0.52
5:J:260:ILE:HA	5:J:300:GLN:O	2.10	0.52
4:B:612:PHE:HZ	5:J:326:HIS:HA	1.75	0.52
4:B:679:GLN:O	4:B:682:GLU:HG2	2.10	0.52
2:D:34:DC:H2"	2:D:35:DC:C5	2.44	0.52
3:I:41:DC:H2'	3:I:42:DC:C6	2.44	0.52
4:B:246:LEU:HD22	4:B:267:VAL:HG21	1.91	0.51
1:G:54:VAL:CG1	1:G:58:LEU:HB3	2.40	0.51
4:A:1205:LYS:HE2	4:A:1209:GLN:NE2	2.25	0.51
4:B:936:ARG:HB2	4:B:1215:GLY:H	1.75	0.51
5:J:162:ILE:O	5:J:163:LYS:HG3	2.11	0.51
4:B:1116:LYS:HG3	4:B:1117:ASN:N	2.25	0.51
4:B:339:LEU:HB3	4:B:343:ASP:HB2	1.92	0.51
4:A:569:LEU:N	4:A:570:PRO:HD2	2.26	0.51
1:C:133:ILE:HG23	1:C:137:HIS:CE1	2.45	0.51
1:C:173:ALA:O	1:C:181:LYS:HE3	2.10	0.51
4:A:1119:PHE:HB3	4:A:1120:PRO:HD3	1.91	0.51
4:A:1155:THR:HB	4:A:1163:MET:SD	2.51	0.51
4:A:339:LEU:HB3	4:A:343:ASP:HB2	1.92	0.51
1:G:154:LYS:HE2	1:G:215:MET:SD	2.50	0.51
1:G:165:TYR:CE1	1:G:192:LEU:HD11	2.46	0.51
2:H:45:DT:H2"	2:H:46:DA:C8	2.46	0.51
5:F:201:LYS:HE2	5:F:236:LYS:NZ	2.26	0.51
4:A:956:TYR:CE1	4:A:991:LYS:HA	2.46	0.51
4:B:961:ALA:O	4:B:964:GLU:HB3	2.11	0.51
3:E:15:DC:H2"	3:E:16:DG:OP1	2.11	0.51
3:E:16:DG:O4'	4:A:616:GLN:HB3	2.10	0.51
5:F:126:ASP:HB3	5:F:129:PHE:CD2	2.46	0.51
4:A:1011:GLU:O	4:A:1015:ARG:HG3	2.11	0.50
4:A:992:GLN:HG3	4:A:1010:ILE:HG12	1.91	0.50
4:B:300:ALA:HB2	4:B:333:LEU:HD11	1.93	0.50
5:F:104:PRO:HG3	5:F:122:ALA:HB1	1.93	0.50
4:B:801:ASP:OD1	4:B:805:ARG:N	2.44	0.50
3:I:25:DT:H2"	3:I:26:DT:H71	1.93	0.50
4:A:994:VAL:HG13	4:A:1040:LEU:HD11	1.94	0.50
4:A:283:VAL:HA	4:A:286:MET:HE3	1.93	0.50
4:A:422:LEU:CG	4:A:427:VAL:HG21	2.41	0.50
4:B:993:THR:HA	4:B:1010:ILE:HD13	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:194:MET:HG2	5:J:228:PHE:CD2	2.46	0.50
4:B:844:HIS:CG	4:B:919:VAL:HG13	2.46	0.50
1:C:225:VAL:HG12	1:C:225:VAL:O	2.11	0.50
5:J:201:LYS:HE3	5:J:233:GLU:OE2	2.11	0.50
4:A:236:THR:CG2	4:A:473:LEU:HD23	2.41	0.50
4:B:1147:VAL:HG23	4:B:1154:TRP:HB2	1.94	0.50
4:A:690:THR:HA	4:A:693:HIS:CE1	2.47	0.50
4:B:919:VAL:O	4:B:1154:TRP:HA	2.12	0.50
4:B:967:ARG:NH2	4:B:982:GLU:HG3	2.27	0.50
4:B:296:LEU:HG	4:B:328:LEU:HD22	1.93	0.50
4:B:618:ILE:HD12	4:B:620:ILE:HG13	1.92	0.50
4:B:1004:TYR:CB	4:B:1007:ARG:HB2	2.42	0.50
4:B:815:HIS:CD2	4:B:1149:VAL:HG22	2.47	0.50
4:B:423:PRO:CD	4:B:427:VAL:HG23	2.42	0.50
2:D:7:DT:H2'	2:D:8:DT:C6	2.47	0.50
3:E:18:DT:H2"	3:E:19:DA:C8	2.47	0.50
3:E:18:DT:H2"	3:E:19:DA:H8	1.77	0.50
1:G:225:VAL:HG12	1:G:225:VAL:O	2.12	0.50
1:G:68:PHE:HB3	1:G:80:LEU:HD22	1.93	0.50
2:D:20:DG:O6	3:E:32:DA:N6	2.45	0.49
3:I:20:DT:H2"	3:I:21:DG:H8	1.75	0.49
4:A:1059:ARG:HG2	4:A:1116:LYS:HB2	1.94	0.49
4:B:569:LEU:N	4:B:570:PRO:HD2	2.27	0.49
4:B:653:LEU:HG	4:B:664:LEU:HD23	1.93	0.49
5:F:164:PRO:CD	5:F:165:PRO:HD2	2.42	0.49
3:I:18:DT:H2"	3:I:19:DA:C8	2.45	0.49
4:A:417:VAL:HG13	4:A:784:SER:HA	1.94	0.49
1:C:133:ILE:O	1:C:137:HIS:ND1	2.42	0.49
3:E:19:DA:H2"	3:E:20:DT:C7	2.42	0.49
1:G:231:LEU:O	1:G:233:ARG:NH1	2.46	0.49
4:A:331:GLN:OE1	4:A:361:PRO:HD3	2.12	0.49
4:B:1147:VAL:CG2	4:B:1154:TRP:HB2	2.43	0.49
2:D:35:DC:OP2	5:F:201:LYS:NZ	2.45	0.49
3:E:16:DG:C4	4:A:616:GLN:HG2	2.47	0.49
1:G:58:LEU:HG	3:I:31:DC:O2	2.13	0.49
4:B:1172:VAL:HG21	4:B:1223:LYS:HG3	1.94	0.49
1:G:78:THR:HG23	2:H:19:DT:C1'	2.42	0.49
2:H:47:DG:H2"	2:H:48:DG:C8	2.47	0.49
4:B:456:LEU:O	4:B:460:VAL:HG23	2.13	0.49
3:I:16:DG:C5	4:B:616:GLN:HG2	2.48	0.49
4:B:962:GLN:O	4:B:965:VAL:HG22	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:VAL:CG1	1:C:58:LEU:HB3	2.43	0.49
1:G:218:TRP:CH2	1:G:222:MET:HG3	2.47	0.49
5:F:85:ALA:O	5:F:89:LEU:HG	2.13	0.49
4:B:990:VAL:O	4:B:994:VAL:HG23	2.12	0.49
3:E:3:DC:H2"	3:E:4:DC:C6	2.48	0.49
5:F:119:LYS:HE3	5:F:143:LYS:HB3	1.95	0.49
4:A:940:GLY:HA2	4:A:1044:PHE:HE1	1.77	0.49
4:B:239:LEU:HD11	4:B:270:GLY:HA3	1.94	0.49
1:C:156:LYS:HD3	2:D:7:DT:H5'	1.95	0.49
1:G:154:LYS:HE2	1:G:215:MET:CE	2.43	0.49
4:A:1004:TYR:CB	4:A:1007:ARG:HB2	2.43	0.49
4:A:1004:TYR:HB3	4:A:1007:ARG:HD2	1.95	0.49
4:B:138:GLN:HA	4:B:141:LYS:HE2	1.95	0.49
4:B:265:ASN:ND2	4:B:298:SER:OG	2.46	0.49
1:C:212:HIS:NE2	1:C:216:LYS:HE3	2.28	0.49
4:B:1084:LEU:HG	4:B:1111:ASN:HB2	1.95	0.48
4:B:591:CYS:SG	4:B:601:ARG:NH2	2.76	0.48
1:G:232:ARG:NH1	3:I:48:DA:OP1	2.36	0.48
4:B:1011:GLU:O	4:B:1015:ARG:HG3	2.14	0.48
4:B:219:LEU:HD12	4:B:224:GLN:NE2	2.28	0.48
3:E:19:DA:H2"	3:E:20:DT:H73	1.94	0.48
3:E:28:DT:H2"	3:E:29:DA:C8	2.48	0.48
5:F:136:LEU:O	5:F:139:ASN:HB2	2.13	0.48
4:A:235:LEU:HD13	4:A:512:HIS:NE2	2.28	0.48
4:B:1120:PRO:CB	4:B:1121:PRO:HD3	2.42	0.48
4:B:547:CYS:SG	4:B:552:TYR:HB2	2.53	0.48
5:F:137:GLY:HA3	5:F:144:LEU:HD23	1.96	0.48
4:A:1083:ARG:HD3	4:A:1107:SER:CB	2.43	0.48
4:A:1149:VAL:HG12	4:A:1150:HIS:CE1	2.48	0.48
4:A:590:PRO:CB	4:A:599:SER:HB3	2.43	0.48
4:B:680:HIS:O	4:B:684:LEU:HG	2.14	0.48
2:H:18:DC:H2"	2:H:19:DT:C6	2.48	0.48
4:A:608:HIS:HA	4:A:620:ILE:O	2.13	0.48
4:B:1082:TYR:HB2	4:B:1115:GLN:HE21	1.79	0.48
4:A:592:SER:O	4:A:593:LEU:HG	2.14	0.48
4:B:815:HIS:HD2	4:B:1149:VAL:HG22	1.79	0.48
4:A:507:ARG:HB3	4:A:511:ARG:NH1	2.29	0.48
1:C:233:ARG:HG2	3:E:49:DC:P	2.54	0.48
5:F:88:TYR:CD1	5:F:192:VAL:HG11	2.48	0.48
5:F:212:TYR:CE1	5:F:253:ILE:HG23	2.49	0.48
4:A:283:VAL:HA	4:A:286:MET:HE2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:419:LYS:HE3	4:B:431:ARG:NH2	2.28	0.47
4:B:799:ASN:O	4:B:806:THR:HA	2.13	0.47
4:B:820:VAL:HG22	4:B:892:TRP:CD1	2.48	0.47
4:B:533:TYR:OH	4:B:549:PRO:HB3	2.13	0.47
4:B:940:GLY:HA2	4:B:1044:PHE:CE1	2.48	0.47
3:E:4:DC:H2"	3:E:5:DT:C6	2.49	0.47
4:A:845:LEU:O	4:A:849:THR:HG23	2.14	0.47
4:B:230:PHE:CD2	4:B:263:MET:HB3	2.48	0.47
4:B:994:VAL:CG1	4:B:998:VAL:HG23	2.44	0.47
4:A:279:GLU:N	4:A:279:GLU:OE1	2.47	0.47
4:B:929:GLN:HA	4:B:944:VAL:HG21	1.96	0.47
3:E:21:DG:C4	3:E:22:DC:C5	3.02	0.47
3:I:17:DG:C2'	3:I:18:DT:H71	2.43	0.47
4:A:802:PHE:O	4:A:1078:VAL:HG13	2.14	0.47
2:D:13:DG:H2"	2:D:14:DG:C8	2.49	0.47
3:E:15:DC:H4'	3:E:16:DG:OP2	2.15	0.47
5:F:260:ILE:HA	5:F:300:GLN:O	2.14	0.47
1:G:106:GLU:HA	1:G:109:VAL:HG12	1.97	0.47
5:F:99:LEU:HD21	5:F:190:LYS:HE3	1.97	0.47
4:A:414:VAL:HG22	4:A:788:HIS:CG	2.50	0.47
4:B:1059:ARG:HG2	4:B:1116:LYS:HD3	1.97	0.47
4:B:948:PRO:HD3	4:B:1221:GLN:HB3	1.96	0.47
5:F:164:PRO:N	5:F:165:PRO:HD2	2.30	0.47
4:A:1003:ARG:HD2	4:A:1114:LYS:NZ	2.29	0.47
4:A:871:ILE:HG23	4:A:898:CYS:SG	2.55	0.47
4:B:456:LEU:HD12	4:B:471:LEU:HD12	1.97	0.47
1:G:166:VAL:HA	1:G:185:VAL:HG11	1.97	0.47
5:J:389:TYR:HB3	5:J:390:ASP:H	1.56	0.47
4:A:948:PRO:HD3	4:A:1221:GLN:HB3	1.97	0.47
2:D:3:DT:C2'	2:D:4:DT:H71	2.44	0.47
5:F:344:PRO:HD3	5:F:388:LEU:HD21	1.97	0.47
5:J:267:PRO:HA	5:J:295:LYS:HA	1.96	0.47
4:A:497:PHE:CD1	4:A:621:LEU:HD11	2.50	0.47
4:A:400:PHE:HE1	4:A:664:LEU:HD13	1.80	0.47
4:A:961:ALA:O	4:A:964:GLU:HB3	2.14	0.47
4:B:658:PRO:HA	4:B:670:LEU:HD22	1.97	0.46
5:F:78:ARG:NH2	5:F:115:GLU:OE1	2.45	0.46
4:A:304:GLN:HG2	4:A:308:ARG:HH12	1.78	0.46
4:A:554:GLU:HA	4:A:558:ALA:HB2	1.96	0.46
4:A:808:PRO:HD3	4:A:816:LEU:HD13	1.97	0.46
1:C:55:SER:HA	1:C:103:TYR:CD1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:380:SER:O	5:F:386:LYS:HE2	2.15	0.46
4:A:467:LEU:HD12	4:A:578:LEU:CD1	2.45	0.46
4:A:993:THR:O	4:A:996:THR:HB	2.14	0.46
4:B:994:VAL:HG12	4:B:998:VAL:HG21	1.97	0.46
1:C:166:VAL:HA	1:C:185:VAL:HG11	1.98	0.46
1:C:107:TRP:CZ2	2:D:24:DA:H5"	2.50	0.46
5:J:256:LEU:O	5:J:307:LEU:HD13	2.16	0.46
4:A:1041:GLN:CD	4:A:1048:ARG:HH11	2.19	0.46
3:E:3:DC:H2"	3:E:4:DC:C5	2.51	0.46
4:A:469:PRO:O	4:A:473:LEU:HG	2.16	0.46
4:B:474:LEU:HD12	4:B:515:GLN:OE1	2.15	0.46
4:B:987:ARG:O	4:B:991:LYS:N	2.39	0.46
1:C:117:PHE:CE2	1:C:121:LEU:HD11	2.49	0.46
2:H:32:DT:H2"	2:H:33:DA:H8	1.81	0.46
5:F:162:ILE:O	5:F:163:LYS:HG3	2.16	0.46
4:A:671:MET:SD	4:A:684:LEU:HD11	2.56	0.46
1:G:154:LYS:HG3	1:G:218:TRP:CD2	2.51	0.46
3:I:15:DC:H4'	3:I:16:DG:OP2	2.16	0.46
5:J:244:PRO:O	5:J:331:ARG:NH2	2.49	0.46
3:I:39:DC:C2	3:I:40:DC:C5	3.04	0.46
4:A:589:MET:HB3	4:A:605:VAL:HG22	1.97	0.46
4:B:709:VAL:HG11	4:B:714:LEU:HD22	1.98	0.46
4:B:846:VAL:HG21	4:B:860:ARG:O	2.16	0.46
4:B:994:VAL:HG12	4:B:998:VAL:HG23	1.98	0.46
3:E:46:DT:H2"	3:E:47:DA:N7	2.31	0.46
1:G:65:LEU:HB3	1:G:66:PRO:HD3	1.97	0.46
4:A:977:VAL:HA	4:A:980:VAL:HG22	1.98	0.45
1:C:77:THR:HB	3:E:33:DG:H21	1.81	0.45
5:F:84:LEU:O	5:F:88:TYR:CD2	2.68	0.45
4:A:1125:HIS:HA	4:A:1128:ASP:OD2	2.15	0.45
4:A:1151:ASP:N	4:A:1151:ASP:OD1	2.48	0.45
4:B:852:LYS:HE3	4:B:863:PHE:CD1	2.51	0.45
4:B:557:GLY:HA3	4:B:558:ALA:HA	1.61	0.45
4:B:847:ASN:OD1	4:B:860:ARG:NH1	2.50	0.45
3:I:3:DC:H2"	3:I:4:DC:C6	2.52	0.45
4:A:808:PRO:CD	4:A:816:LEU:HD13	2.46	0.45
4:B:419:LYS:HE2	4:B:422:LEU:CD1	2.46	0.45
4:B:497:PHE:CE2	4:B:577:LYS:HG2	2.52	0.45
1:C:233:ARG:HG2	3:E:49:DC:OP1	2.16	0.45
5:F:137:GLY:O	5:F:141:ASP:N	2.28	0.45
5:F:244:PRO:HB3	5:F:363:VAL:CG2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1150:HIS:CD2	4:A:1151:ASP:H	2.35	0.45
1:C:164:VAL:HG13	4:A:122:TRP:CZ2	2.51	0.45
4:B:1205:LYS:HE2	4:B:1209:GLN:NE2	2.31	0.45
5:F:335:VAL:CG1	5:F:351:LEU:HD21	2.46	0.45
4:A:523:VAL:O	4:A:527:GLN:HG3	2.17	0.45
1:C:65:LEU:HB3	1:C:66:PRO:HD3	1.98	0.45
4:A:426:GLU:OE2	4:A:633:LYS:HG2	2.17	0.45
3:I:41:DC:H2"	3:I:42:DC:O5'	2.16	0.45
5:J:212:TYR:CE1	5:J:253:ILE:HG23	2.52	0.45
4:B:516:ARG:HH22	4:B:562:LEU:HD22	1.82	0.45
1:C:78:THR:HA	2:D:19:DT:H1'	1.99	0.45
4:A:397:GLN:O	4:A:401:GLU:HG2	2.17	0.45
4:A:456:LEU:HD22	4:A:466:SER:HB2	1.99	0.45
4:B:225:ARG:HD2	4:B:465:PHE:CE1	2.52	0.45
4:B:995:MET:O	4:B:999:TYR:HD1	2.00	0.45
2:D:17:DA:H2"	2:D:18:DC:C6	2.51	0.45
3:E:17:DG:OP2	4:A:1100:TYR:HA	2.16	0.45
3:E:39:DC:C4	3:E:40:DC:N4	2.85	0.45
4:A:497:PHE:HD1	4:A:621:LEU:HD11	1.81	0.45
4:A:438:ARG:NH1	4:A:636:GLU:OE2	2.35	0.45
4:A:680:HIS:O	4:A:684:LEU:HG	2.15	0.45
1:C:106:GLU:HA	1:C:109:VAL:HG12	1.98	0.45
3:I:2:DG:H2"	3:I:3:DC:C6	2.52	0.45
5:J:164:PRO:CD	5:J:165:PRO:HD2	2.47	0.45
4:A:419:LYS:HE3	4:A:431:ARG:HH22	1.81	0.44
4:A:712:ARG:NH2	4:A:875:ALA:O	2.43	0.44
4:B:523:VAL:O	4:B:527:GLN:HG3	2.17	0.44
3:I:14:DG:H22	4:B:1102:HIS:HA	1.82	0.44
4:A:222:GLN:NE2	4:A:225:ARG:HH21	2.15	0.44
5:J:164:PRO:N	5:J:165:PRO:HD2	2.33	0.44
4:A:1059:ARG:HE	4:A:1116:LYS:HD2	1.83	0.44
4:B:236:THR:HG23	4:B:473:LEU:HD23	2.00	0.44
4:B:419:LYS:NZ	4:B:422:LEU:HD22	2.32	0.44
3:E:16:DG:C8	3:E:16:DG:OP1	2.70	0.44
4:A:718:LEU:HB3	4:A:722:GLN:NE2	2.32	0.44
4:B:612:PHE:CZ	5:J:326:HIS:HA	2.53	0.44
3:I:24:DC:H2"	3:I:25:DT:C6	2.53	0.44
4:B:419:LYS:HE2	4:B:422:LEU:HD13	1.99	0.44
1:C:54:VAL:HG22	3:E:31:DC:H5'	2.00	0.44
5:J:140:LEU:N	5:J:140:LEU:HD23	2.31	0.44
4:A:265:ASN:HB3	4:A:297:LEU:HD23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:445:LEU:HD21	4:A:583:LEU:HD12	1.99	0.44
4:B:844:HIS:CD2	4:B:920:HIS:H	2.36	0.44
2:D:32:DT:H2"	2:D:33:DA:C8	2.53	0.44
1:G:211:TYR:CZ	1:G:215:MET:HG3	2.52	0.44
5:J:312:LEU:HD23	5:J:371:LYS:HE3	1.99	0.44
2:D:2:DG:C8	2:D:3:DT:H72	2.53	0.44
1:G:61:SER:HA	1:G:84:ILE:HG21	2.00	0.44
4:A:1059:ARG:HG2	4:A:1116:LYS:CB	2.47	0.44
4:B:464:ARG:NH1	4:B:465:PHE:H	2.16	0.44
4:B:670:LEU:HD23	4:B:684:LEU:HD13	2.00	0.44
1:C:205:LYS:O	1:C:208:GLU:HB2	2.18	0.44
4:A:590:PRO:HB3	4:A:599:SER:HB3	1.98	0.43
1:C:167:ALA:HB3	4:A:122:TRP:CH2	2.53	0.43
4:A:1059:ARG:NE	4:A:1116:LYS:HD2	2.33	0.43
4:A:363:GLN:HB3	4:A:364:LEU:CA	2.49	0.43
4:B:852:LYS:HE3	4:B:863:PHE:CG	2.52	0.43
1:C:160:SER:O	1:C:164:VAL:HG23	2.18	0.43
3:E:4:DC:H2'	3:E:5:DT:H72	1.99	0.43
5:F:140:LEU:HD23	5:F:140:LEU:N	2.32	0.43
3:I:41:DC:H2"	3:I:42:DC:C5'	2.48	0.43
4:A:1059:ARG:CG	4:A:1116:LYS:HB2	2.48	0.43
4:A:411:ARG:NH1	4:A:511:ARG:HH21	2.16	0.43
4:B:1015:ARG:NH2	4:B:1025:VAL:HG11	2.33	0.43
4:B:601:ARG:NH1	5:J:346:ASP:HB2	2.33	0.43
4:A:126:LEU:O	4:A:130:LYS:HG3	2.18	0.43
4:A:941:ALA:HA	4:A:946:LEU:HB2	2.01	0.43
4:B:1015:ARG:HG3	4:B:1025:VAL:HG21	2.00	0.43
1:C:155:PRO:HG2	1:C:214:GLU:HB3	2.00	0.43
1:C:153:GLY:O	1:C:218:TRP:CD1	2.72	0.43
2:D:21:DT:C2'	2:D:22:DT:H71	2.49	0.43
3:E:17:DG:H2'	3:E:18:DT:H71	1.99	0.43
4:B:936:ARG:HB2	4:B:1215:GLY:N	2.32	0.43
3:E:19:DA:C8	3:E:20:DT:H72	2.53	0.43
5:F:164:PRO:HG2	5:F:165:PRO:CD	2.48	0.43
5:F:244:PRO:HB3	5:F:363:VAL:HG21	1.99	0.43
4:A:870:ASP:OD1	4:A:882:ARG:NH1	2.50	0.43
1:C:147:LYS:O	1:C:151:LEU:HD13	2.17	0.43
5:J:239:ALA:HB2	5:J:246:LEU:HB2	2.01	0.43
4:A:1043:MET:HG3	4:A:1044:PHE:CE2	2.53	0.43
4:A:931:TYR:CZ	4:A:1051:GLN:HG2	2.54	0.43
4:A:990:VAL:O	4:A:994:VAL:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1123:PHE:CE2	4:B:1127:LEU:HD11	2.54	0.43
4:B:1188:VAL:O	4:B:1192:CYS:HB2	2.18	0.43
4:B:452:THR:HG23	4:B:455:ARG:NH2	2.34	0.43
1:C:107:TRP:O	1:C:111:LYS:HG3	2.18	0.43
3:E:16:DG:H2"	3:E:17:DG:C8	2.54	0.43
4:A:1196:GLN:HA	4:A:1197:LYS:HA	1.75	0.43
4:B:491:PRO:HG2	4:B:494:GLY:O	2.19	0.43
5:J:78:ARG:NH2	5:J:115:GLU:OE1	2.49	0.43
5:J:249:VAL:HG13	5:J:324:LEU:HB3	2.01	0.43
4:A:1024:PHE:O	4:A:1028:ALA:N	2.37	0.43
4:A:1150:HIS:HE2	4:A:1152:CYS:HG	1.61	0.43
4:B:618:ILE:HD11	4:B:620:ILE:HD11	2.01	0.43
2:D:16:DG:H2"	2:D:17:DA:C8	2.54	0.43
1:G:218:TRP:CZ3	1:G:222:MET:HG3	2.54	0.43
5:J:98:LEU:O	5:J:189:LEU:HD12	2.18	0.43
4:A:241:LEU:HD11	4:A:460:VAL:HG11	2.00	0.42
1:C:218:TRP:HH2	1:C:230:LEU:HD13	1.83	0.42
2:D:36:DT:C2	4:A:615:VAL:HG11	2.54	0.42
4:A:1001:VAL:HG12	4:A:1002:THR:HG23	2.00	0.42
4:A:589:MET:HG2	4:A:605:VAL:HG22	2.00	0.42
4:A:961:ALA:O	4:A:965:VAL:HG13	2.19	0.42
2:H:48:DG:H2"	2:H:49:DC:C6	2.54	0.42
5:J:248:HIS:CE1	5:J:331:ARG:NH1	2.87	0.42
4:A:1072:THR:CG2	4:A:1126:SER:HB2	2.45	0.42
2:D:48:DG:H2"	2:D:49:DC:C6	2.54	0.42
5:F:346:ASP:HB3	5:F:349:ASP:HB3	2.01	0.42
4:B:845:LEU:O	4:B:849:THR:HG23	2.19	0.42
5:F:149:CYS:SG	5:F:154:LEU:HD21	2.59	0.42
4:B:456:LEU:HD22	4:B:466:SER:HB2	2.01	0.42
4:B:497:PHE:HE2	4:B:577:LYS:HG2	1.85	0.42
1:G:100:GLN:O	1:G:104:ARG:HG3	2.19	0.42
5:J:205:TRP:CE2	5:J:250:LEU:HD21	2.53	0.42
4:B:1013:ARG:HH21	4:B:1016:GLU:CD	2.23	0.42
1:G:164:VAL:HG13	4:B:122:TRP:CZ2	2.55	0.42
2:H:46:DA:H2"	2:H:47:DG:C8	2.54	0.42
4:A:132:THR:O	4:A:136:ARG:HG3	2.20	0.42
4:B:510:SER:O	4:B:514:VAL:HG23	2.19	0.42
1:C:103:TYR:OH	2:D:23:DA:H4'	2.20	0.42
1:C:100:GLN:O	1:C:104:ARG:HG3	2.19	0.42
1:C:117:PHE:CZ	1:C:121:LEU:HD21	2.55	0.42
4:A:601:ARG:NH1	5:F:346:ASP:HB2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1053:TRP:CZ2	4:A:1211:VAL:HG22	2.55	0.42
4:A:619:GLY:O	4:A:620:ILE:HD13	2.20	0.42
4:B:870:ASP:OD1	4:B:882:ARG:NH1	2.53	0.42
1:C:164:VAL:HG12	1:C:200:TYR:HD1	1.85	0.42
1:C:155:PRO:HG2	1:C:214:GLU:CB	2.50	0.42
1:G:170:PHE:HA	1:G:185:VAL:HG21	2.01	0.42
3:I:20:DT:C2	3:I:21:DG:N7	2.88	0.42
4:A:363:GLN:CB	4:A:364:LEU:HA	2.49	0.42
4:A:992:GLN:HG3	4:A:1010:ILE:CG1	2.50	0.42
4:B:279:GLU:OE1	4:B:279:GLU:N	2.50	0.42
4:B:369:ASN:HB3	4:B:378:TYR:CD2	2.54	0.42
2:D:18:DC:H2"	2:D:19:DT:C6	2.55	0.42
3:E:22:DC:H2"	3:E:23:DA:C8	2.55	0.42
4:A:229:PHE:HB2	4:A:465:PHE:HE2	1.85	0.42
4:A:589:MET:CG	4:A:605:VAL:HG22	2.50	0.42
1:C:222:MET:HE2	1:C:230:LEU:HD12	2.01	0.42
4:A:838:LEU:HG	4:A:842:LYS:HE3	2.02	0.41
1:G:91:LEU:HG	1:G:95:LYS:HB2	2.02	0.41
3:I:16:DG:H8	3:I:16:DG:OP1	2.03	0.41
4:A:241:LEU:HD11	4:A:460:VAL:CG1	2.50	0.41
4:A:563:ARG:HD3	4:A:659:HIS:CD2	2.54	0.41
4:B:276:ALA:HB1	4:B:279:GLU:OE1	2.20	0.41
4:B:232:CYS:SG	4:B:469:PRO:HB2	2.60	0.41
5:J:346:ASP:HB3	5:J:349:ASP:HB3	2.02	0.41
4:A:996:THR:OG1	4:A:1010:ILE:HD11	2.21	0.41
4:A:1023:GLU:HG3	4:A:1024:PHE:CD2	2.55	0.41
2:D:3:DT:H2"	2:D:4:DT:H71	2.01	0.41
5:F:114:LEU:HD22	5:F:140:LEU:HD12	2.02	0.41
1:G:45:VAL:HB	1:G:129:LEU:HB2	2.01	0.41
4:A:127:GLU:O	4:A:131:ARG:HG3	2.21	0.41
4:A:304:GLN:HG3	4:A:346:THR:OG1	2.20	0.41
4:A:995:MET:O	4:A:999:TYR:HB2	2.21	0.41
4:B:368:VAL:HG11	4:B:380:LYS:NZ	2.35	0.41
4:B:389:LEU:HD12	4:B:537:LEU:HB3	2.02	0.41
4:B:716:LEU:HD11	4:B:878:PRO:HG2	2.01	0.41
3:E:20:DT:C2	3:E:21:DG:N7	2.89	0.41
4:A:366:PRO:HA	4:A:367:PRO:HD3	1.94	0.41
4:A:399:LEU:HB3	4:A:649:LEU:O	2.19	0.41
4:A:808:PRO:HG3	4:A:815:HIS:CE1	2.55	0.41
3:E:15:DC:H6	3:E:15:DC:H2'	1.68	0.41
4:A:124:LYS:O	4:A:128:LYS:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:422:LEU:CD2	4:B:427:VAL:HG11	2.39	0.41
3:E:4:DC:C2'	3:E:5:DT:H72	2.51	0.41
5:F:167:MET:HE2	5:F:172:LEU:HB2	2.02	0.41
4:A:547:CYS:SG	4:A:552:TYR:HB2	2.61	0.41
4:A:557:GLY:HA3	4:A:558:ALA:HA	1.45	0.41
4:B:371:SER:HB3	4:B:374:LEU:HB2	2.02	0.41
4:B:530:TYR:HA	4:B:553:TRP:HZ3	1.86	0.41
4:B:922:ASP:OD1	4:B:1152:CYS:HB3	2.21	0.41
1:C:211:TYR:CZ	1:C:215:MET:HG3	2.55	0.41
1:G:165:TYR:CD2	1:G:189:TRP:HB2	2.55	0.41
2:H:17:DA:H2"	2:H:18:DC:C6	2.55	0.41
5:J:192:VAL:HA	5:J:226:ASN:O	2.21	0.41
4:A:136:ARG:O	4:A:140:LEU:HG	2.21	0.41
3:E:16:DG:C4	4:A:616:GLN:CG	3.03	0.41
4:A:852:LYS:HD2	4:A:855:GLU:HG3	2.03	0.41
4:B:363:GLN:HB3	4:B:364:LEU:CA	2.51	0.41
4:B:438:ARG:HH22	4:B:636:GLU:CD	2.23	0.41
1:C:52:LYS:NZ	3:E:29:DA:N3	2.69	0.41
5:J:205:TRP:CD2	5:J:250:LEU:HD21	2.56	0.41
4:A:374:LEU:HB3	4:A:378:TYR:CE2	2.56	0.41
3:E:19:DA:C4	3:E:20:DT:H72	2.56	0.41
5:F:330:ARG:HB2	5:F:338:HIS:CE1	2.55	0.41
4:A:625:PRO:HB2	5:F:385:TYR:CZ	2.55	0.41
4:B:224:GLN:OE1	4:B:568:PRO:HB3	2.21	0.41
1:G:152:LEU:N	1:G:152:LEU:HD12	2.36	0.41
5:J:194:MET:HG2	5:J:228:PHE:HD2	1.85	0.41
4:A:246:LEU:HD22	4:A:267:VAL:CG2	2.46	0.41
4:B:653:LEU:HG	4:B:664:LEU:CD2	2.50	0.41
2:D:30:DC:H2"	2:D:31:DA:C8	2.56	0.41
1:G:58:LEU:HG	3:I:31:DC:C2	2.55	0.41
5:J:136:LEU:O	5:J:139:ASN:HB2	2.21	0.41
4:A:387:PRO:HD3	4:A:1143:GLY:HA2	2.03	0.40
4:B:334:PHE:CE1	4:B:348:LEU:HG	2.56	0.40
5:F:248:HIS:CE1	5:F:331:ARG:HH12	2.39	0.40
5:J:193:GLY:O	5:J:227:MET:HA	2.21	0.40
4:A:1170:GLN:HE22	4:A:1173:ARG:NH1	2.20	0.40
4:A:300:ALA:HB2	4:A:333:LEU:HD11	2.02	0.40
4:A:801:ASP:OD1	4:A:805:ARG:N	2.54	0.40
4:A:799:ASN:O	4:A:806:THR:HA	2.21	0.40
4:B:343:ASP:O	4:B:347:VAL:HG23	2.21	0.40
4:B:412:VAL:HG21	4:B:646:VAL:HG21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:822:ARG:NH2	4:A:1150:HIS:HE1	2.19	0.40
4:A:455:ARG:O	4:A:459:GLU:HG3	2.20	0.40
1:C:188:ASN:O	1:C:192:LEU:HG	2.21	0.40
2:D:32:DT:H2"	2:D:33:DA:H8	1.85	0.40
1:G:232:ARG:HA	3:I:49:DC:OP1	2.21	0.40
4:A:1080:GLN:HA	4:A:1081:PRO:HD3	1.88	0.40
4:A:343:ASP:O	4:A:347:VAL:HG23	2.21	0.40
5:F:127:LYS:HG3	5:F:130:ILE:HD12	2.04	0.40
3:I:21:DG:C4	3:I:22:DC:C5	3.10	0.40
3:I:17:DG:H2"	3:I:18:DT:H71	2.03	0.40
3:I:31:DC:N4	3:I:32:DA:H62	2.20	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	
1	C	190/205 (93%)	184 (97%)	6 (3%)	0	100	100
1	G	190/205 (93%)	187 (98%)	3 (2%)	0	100	100
4	A	1001/1128 (89%)	962 (96%)	39 (4%)	0	100	100
4	B	991/1128 (88%)	958 (97%)	33 (3%)	0	100	100
5	F	282/377 (75%)	271 (96%)	11 (4%)	0	100	100
5	J	282/377 (75%)	272 (96%)	10 (4%)	0	100	100
All	All	2936/3420 (86%)	2834 (96%)	102 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	178/188 (95%)	177 (99%)	1 (1%)	86	92
1	G	178/188 (95%)	177 (99%)	1 (1%)	86	92
4	A	865/976 (89%)	859 (99%)	6 (1%)	84	90
4	B	860/976 (88%)	853 (99%)	7 (1%)	81	89
5	F	255/335 (76%)	254 (100%)	1 (0%)	91	94
5	J	255/335 (76%)	253 (99%)	2 (1%)	81	89
All	All	2591/2998 (86%)	2573 (99%)	18 (1%)	84	90

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	151	LEU
1	G	58	LEU
4	A	593	LEU
4	A	612	PHE
4	A	614	ASN
4	A	680	HIS
4	A	965	VAL
4	A	1151	ASP
4	B	593	LEU
4	B	612	PHE
4	B	614	ASN
4	B	680	HIS
4	B	965	VAL
4	B	977	VAL
4	B	1108	ARG
5	F	157	ARG
5	J	157	ARG
5	J	388	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	222	GLN
4	A	252	GLN
4	A	254	GLN
4	A	363	GLN
4	A	565	GLN
4	A	608	HIS
4	A	722	GLN
4	A	815	HIS
4	A	893	GLN
4	A	1035	GLN
4	A	1125	HIS
4	B	222	GLN
4	B	254	GLN
4	B	265	ASN
4	B	363	GLN
4	B	608	HIS
4	B	893	GLN
4	B	969	GLN
4	B	1063	HIS
4	B	1125	HIS
5	F	248	HIS
5	J	148	HIS
5	J	248	HIS

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	C	192/205 (93%)	0.02	10 (5%)	27	24	312, 394, 446, 483	0
1	G	192/205 (93%)	0.23	15 (7%)	13	11	405, 477, 524, 533	0
2	D	46/50 (92%)	-0.17	1 (2%)	62	52	337, 410, 526, 562	0
2	H	46/50 (92%)	-0.02	1 (2%)	62	52	415, 474, 534, 545	0
3	E	45/50 (90%)	-0.16	1 (2%)	62	52	359, 433, 502, 518	0
3	I	45/50 (90%)	-0.05	2 (4%)	34	28	413, 483, 558, 625	0
4	A	1011/1128 (89%)	0.16	45 (4%)	33	28	246, 329, 411, 462	0
4	B	1003/1128 (88%)	0.05	24 (2%)	59	49	269, 356, 432, 478	0
5	F	288/377 (76%)	-0.04	12 (4%)	36	30	287, 345, 461, 501	0
5	J	288/377 (76%)	0.07	12 (4%)	36	30	325, 411, 582, 648	0
All	All	3156/3620 (87%)	0.08	123 (3%)	39	31	246, 362, 500, 648	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	38	DT	5.7
4	A	379	ALA	5.6
4	A	358	PHE	5.6
3	I	14	DG	5.1
4	B	384	VAL	4.9
3	E	14	DG	4.8
1	G	68	PHE	4.2
1	C	197	LYS	4.0
4	A	610	TYR	3.9
3	I	15	DC	3.8
4	A	1145	THR	3.8
4	A	1192	CYS	3.8
1	G	87	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
4	A	1196	GLN	3.7
1	G	69	LYS	3.7
4	A	1099	THR	3.6
4	A	1101	THR	3.5
4	A	1155	THR	3.5
5	F	119	LYS	3.5
4	A	1064	MET	3.4
4	A	1144	LEU	3.4
5	J	73	ARG	3.4
1	G	129	LEU	3.4
4	A	1086	SER	3.4
5	F	159	GLY	3.4
5	J	183	TRP	3.3
5	J	178	ILE	3.3
4	A	1068	VAL	3.2
1	C	174	LYS	3.2
4	A	1069	GLU	3.1
4	B	977	VAL	3.1
5	F	146	VAL	3.1
5	F	160	GLY	3.1
2	H	9	DG	3.1
4	B	382	GLY	3.1
5	F	120	VAL	3.0
4	B	131	ARG	3.0
4	B	134	GLN	3.0
4	B	127	GLU	2.9
1	C	143	MET	2.9
4	B	811	PRO	2.9
4	B	381	ASP	2.9
4	A	253	ARG	2.9
4	A	599	SER	2.9
4	A	761	GLU	2.9
1	G	83	ARG	2.8
4	A	811	PRO	2.8
4	B	380	LYS	2.8
4	A	1141	ARG	2.8
5	F	118	ALA	2.8
5	J	90	GLY	2.8
4	B	546	PRO	2.8
4	B	386	TYR	2.8
1	C	139	LYS	2.8
1	C	138	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
4	B	598	ARG	2.7
4	A	328	LEU	2.7
5	J	111	GLN	2.7
1	G	65	LEU	2.7
4	A	1102	HIS	2.7
5	F	263	LEU	2.7
1	G	43	SER	2.6
4	A	1029	SER	2.6
4	B	904	ALA	2.6
1	G	64	GLN	2.6
4	A	590	PRO	2.6
4	A	981	LEU	2.6
4	A	1036	VAL	2.6
1	C	135	ASP	2.5
4	B	1141	ARG	2.5
5	J	254	TRP	2.5
4	B	421	THR	2.5
5	J	110	THR	2.5
5	J	144	LEU	2.5
5	J	99	LEU	2.5
1	G	75	ALA	2.5
4	A	1033	VAL	2.5
4	B	383	ARG	2.5
4	A	1156	HIS	2.5
4	B	562	LEU	2.5
5	J	200	GLU	2.5
4	B	330	LEU	2.5
4	A	609	VAL	2.4
4	A	1191	PHE	2.4
4	A	1157	ALA	2.4
1	G	133	ILE	2.4
4	A	1197	LYS	2.4
4	B	765	CYS	2.4
1	G	85	ALA	2.4
4	B	422	LEU	2.4
4	A	985	ILE	2.4
4	B	547	CYS	2.4
1	G	136	LYS	2.3
1	G	67	ILE	2.3
1	C	137	HIS	2.3
4	A	378	TYR	2.3
5	F	73	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
4	A	1032	LEU	2.3
4	A	384	VAL	2.3
5	J	121	VAL	2.3
5	J	195	PHE	2.3
4	A	296	LEU	2.3
4	A	333	LEU	2.3
1	C	189	TRP	2.2
5	F	390	ASP	2.2
4	A	817	GLY	2.2
1	G	166	VAL	2.2
4	A	1103	ASN	2.2
4	A	675	GLU	2.2
1	C	142	ALA	2.2
4	A	963	VAL	2.2
5	F	167	MET	2.1
4	B	420	PRO	2.1
4	A	542	GLU	2.1
4	A	382	GLY	2.1
1	G	140	ARG	2.1
4	A	1000	GLY	2.0
4	B	368	VAL	2.0
4	B	1028	ALA	2.0
5	F	158	SER	2.0
1	C	169	ARG	2.0
5	F	72	LYS	2.0
4	A	1200	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.