



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 09:22 am BST

PDB ID : 6C31
Title : Crystal structure of TetR family protein Rv0078 in complex with DNA
Authors : Hsu, H.C.; Li, H.
Deposited on : 2018-01-09
Resolution : 3.00 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

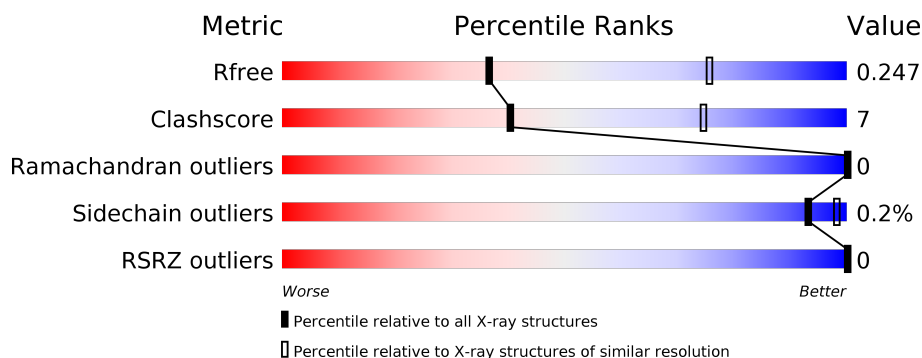
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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.







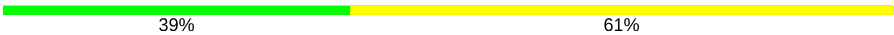

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	214	
1	B	214	
1	C	214	
1	D	214	
1	E	214	
1	F	214	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	214	
1	H	214	
2	I	23	
2	K	23	
3	J	23	
3	L	23	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13639 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 protein called TetR family transcriptional regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	195	Total	C	N	O	S	0	0	0
			1489	929	277	277	6			
1	B	195	Total	C	N	O	S	0	0	0
			1489	929	277	277	6			
1	C	194	Total	C	N	O	S	0	0	0
			1478	923	273	276	6			
1	D	194	Total	C	N	O	S	0	0	0
			1478	923	273	276	6			
1	E	195	Total	C	N	O	S	0	0	0
			1489	929	277	277	6			
1	F	195	Total	C	N	O	S	0	0	0
			1489	929	277	277	6			
1	G	195	Total	C	N	O	S	0	0	0
			1489	929	277	277	6			
1	H	194	Total	C	N	O	S	0	0	0
			1478	923	273	276	6			

There are 104 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	202	LYS	-	expression tag	UNP L0T5M0
A	203	LEU	-	expression tag	UNP L0T5M0
A	204	ALA	-	expression tag	UNP L0T5M0
A	205	ALA	-	expression tag	UNP L0T5M0
A	206	ALA	-	expression tag	UNP L0T5M0
A	207	LEU	-	expression tag	UNP L0T5M0
A	208	GLU	-	expression tag	UNP L0T5M0
A	209	HIS	-	expression tag	UNP L0T5M0
A	210	HIS	-	expression tag	UNP L0T5M0
A	211	HIS	-	expression tag	UNP L0T5M0
A	212	HIS	-	expression tag	UNP L0T5M0
A	213	HIS	-	expression tag	UNP L0T5M0
A	214	HIS	-	expression tag	UNP L0T5M0

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	202	LYS	-	expression tag	UNP L0T5M0
B	203	LEU	-	expression tag	UNP L0T5M0
B	204	ALA	-	expression tag	UNP L0T5M0
B	205	ALA	-	expression tag	UNP L0T5M0
B	206	ALA	-	expression tag	UNP L0T5M0
B	207	LEU	-	expression tag	UNP L0T5M0
B	208	GLU	-	expression tag	UNP L0T5M0
B	209	HIS	-	expression tag	UNP L0T5M0
B	210	HIS	-	expression tag	UNP L0T5M0
B	211	HIS	-	expression tag	UNP L0T5M0
B	212	HIS	-	expression tag	UNP L0T5M0
B	213	HIS	-	expression tag	UNP L0T5M0
B	214	HIS	-	expression tag	UNP L0T5M0
C	202	LYS	-	expression tag	UNP L0T5M0
C	203	LEU	-	expression tag	UNP L0T5M0
C	204	ALA	-	expression tag	UNP L0T5M0
C	205	ALA	-	expression tag	UNP L0T5M0
C	206	ALA	-	expression tag	UNP L0T5M0
C	207	LEU	-	expression tag	UNP L0T5M0
C	208	GLU	-	expression tag	UNP L0T5M0
C	209	HIS	-	expression tag	UNP L0T5M0
C	210	HIS	-	expression tag	UNP L0T5M0
C	211	HIS	-	expression tag	UNP L0T5M0
C	212	HIS	-	expression tag	UNP L0T5M0
C	213	HIS	-	expression tag	UNP L0T5M0
C	214	HIS	-	expression tag	UNP L0T5M0
D	202	LYS	-	expression tag	UNP L0T5M0
D	203	LEU	-	expression tag	UNP L0T5M0
D	204	ALA	-	expression tag	UNP L0T5M0
D	205	ALA	-	expression tag	UNP L0T5M0
D	206	ALA	-	expression tag	UNP L0T5M0
D	207	LEU	-	expression tag	UNP L0T5M0
D	208	GLU	-	expression tag	UNP L0T5M0
D	209	HIS	-	expression tag	UNP L0T5M0
D	210	HIS	-	expression tag	UNP L0T5M0
D	211	HIS	-	expression tag	UNP L0T5M0
D	212	HIS	-	expression tag	UNP L0T5M0
D	213	HIS	-	expression tag	UNP L0T5M0
D	214	HIS	-	expression tag	UNP L0T5M0
E	202	LYS	-	expression tag	UNP L0T5M0
E	203	LEU	-	expression tag	UNP L0T5M0
E	204	ALA	-	expression tag	UNP L0T5M0

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	205	ALA	-	expression tag	UNP L0T5M0
E	206	ALA	-	expression tag	UNP L0T5M0
E	207	LEU	-	expression tag	UNP L0T5M0
E	208	GLU	-	expression tag	UNP L0T5M0
E	209	HIS	-	expression tag	UNP L0T5M0
E	210	HIS	-	expression tag	UNP L0T5M0
E	211	HIS	-	expression tag	UNP L0T5M0
E	212	HIS	-	expression tag	UNP L0T5M0
E	213	HIS	-	expression tag	UNP L0T5M0
E	214	HIS	-	expression tag	UNP L0T5M0
F	202	LYS	-	expression tag	UNP L0T5M0
F	203	LEU	-	expression tag	UNP L0T5M0
F	204	ALA	-	expression tag	UNP L0T5M0
F	205	ALA	-	expression tag	UNP L0T5M0
F	206	ALA	-	expression tag	UNP L0T5M0
F	207	LEU	-	expression tag	UNP L0T5M0
F	208	GLU	-	expression tag	UNP L0T5M0
F	209	HIS	-	expression tag	UNP L0T5M0
F	210	HIS	-	expression tag	UNP L0T5M0
F	211	HIS	-	expression tag	UNP L0T5M0
F	212	HIS	-	expression tag	UNP L0T5M0
F	213	HIS	-	expression tag	UNP L0T5M0
F	214	HIS	-	expression tag	UNP L0T5M0
G	202	LYS	-	expression tag	UNP L0T5M0
G	203	LEU	-	expression tag	UNP L0T5M0
G	204	ALA	-	expression tag	UNP L0T5M0
G	205	ALA	-	expression tag	UNP L0T5M0
G	206	ALA	-	expression tag	UNP L0T5M0
G	207	LEU	-	expression tag	UNP L0T5M0
G	208	GLU	-	expression tag	UNP L0T5M0
G	209	HIS	-	expression tag	UNP L0T5M0
G	210	HIS	-	expression tag	UNP L0T5M0
G	211	HIS	-	expression tag	UNP L0T5M0
G	212	HIS	-	expression tag	UNP L0T5M0
G	213	HIS	-	expression tag	UNP L0T5M0
G	214	HIS	-	expression tag	UNP L0T5M0
H	202	LYS	-	expression tag	UNP L0T5M0
H	203	LEU	-	expression tag	UNP L0T5M0
H	204	ALA	-	expression tag	UNP L0T5M0
H	205	ALA	-	expression tag	UNP L0T5M0
H	206	ALA	-	expression tag	UNP L0T5M0
H	207	LEU	-	expression tag	UNP L0T5M0

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	208	GLU	-	expression tag	UNP L0T5M0
H	209	HIS	-	expression tag	UNP L0T5M0
H	210	HIS	-	expression tag	UNP L0T5M0
H	211	HIS	-	expression tag	UNP L0T5M0
H	212	HIS	-	expression tag	UNP L0T5M0
H	213	HIS	-	expression tag	UNP L0T5M0
H	214	HIS	-	expression tag	UNP L0T5M0

- Molecule 2 is a DNA chain called DNA (5'-D(P*AP*CP*AP*AP*GP*CP*AP*GP*AP*CP*TP*GP*CP*CP*GP*GP*TP*AP*AP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	20	Total	C	N	O	P	0	0	0
			411	194	82	115	20			
2	K	20	Total	C	N	O	P	0	0	0
			411	194	82	115	20			

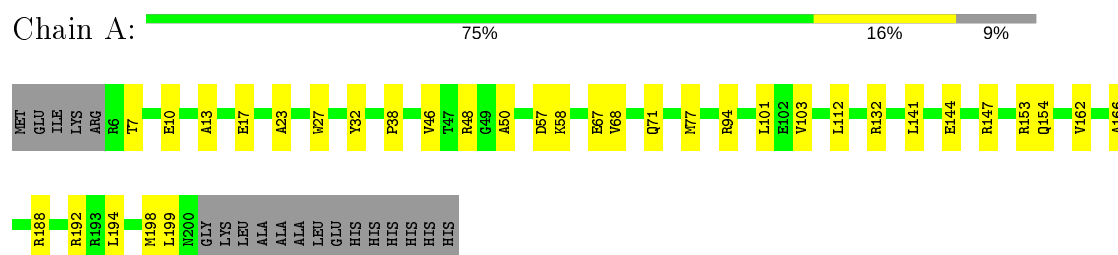
- Molecule 3 is a DNA chain called DNA (5'-D(*GP*TP*TP*AP*CP*CP*GP*GP*CP*AP*GP*TP*CP*TP*GP*CP*TP*TP*GP*TP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	J	23	Total	C	N	O	P	0	0	0
			469	225	84	138	22			
3	L	23	Total	C	N	O	P	0	0	0
			469	225	84	138	22			

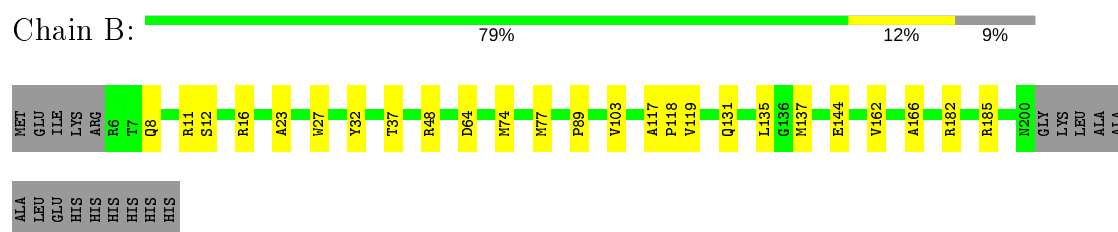
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

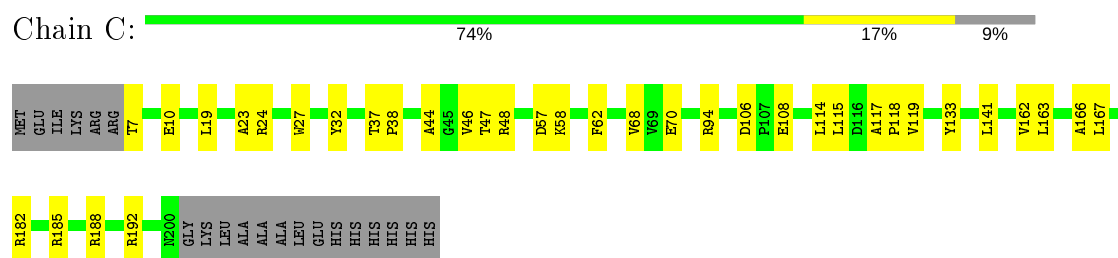
- Molecule 1: TetR family transcriptional regulator



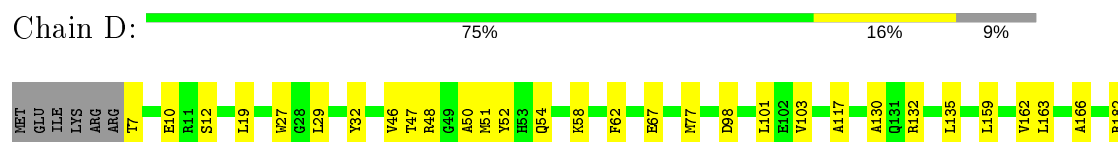
- Molecule 1: TetR family transcriptional regulator

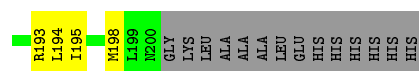


- Molecule 1: TetR family transcriptional regulator



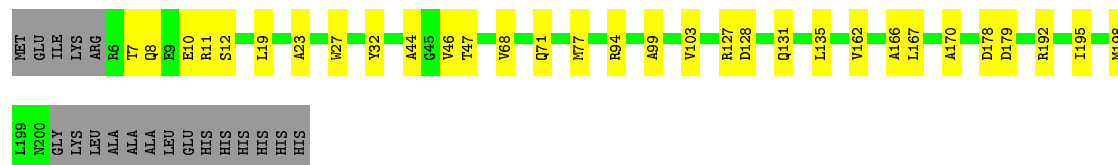
- Molecule 1: TetR family transcriptional regulator





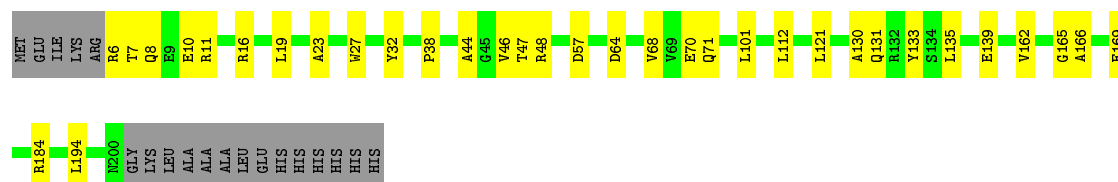
- Molecule 1: TetR family transcriptional regulator

Chain E: 77% 14% 9%



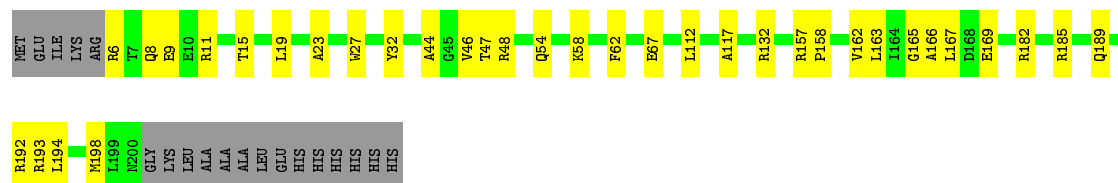
- Molecule 1: TetR family transcriptional regulator

Chain F: 75% 16% 9%



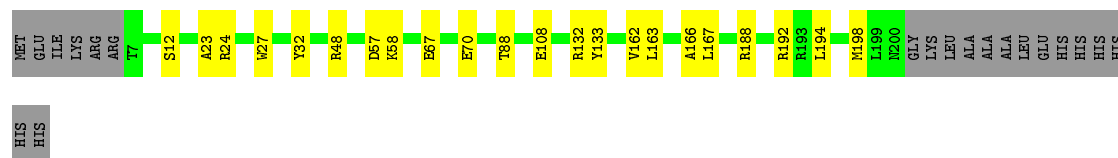
- Molecule 1: TetR family transcriptional regulator

Chain G: 75% 16% 9%



- Molecule 1: TetR family transcriptional regulator

Chain H: 80% 10% 9%



- Molecule 2: DNA (5'-D(P*AP*CP*AP*AP*GP*CP*AP*GP*AP*CP*TP*GP*CP*CP*GP*GP*TP*AP*AP*C)-3')

Chain I: 48% 30% 9% 13%



- Molecule 2: DNA (5'-D(P*AP*CP*AP*AP*GP*CP*AP*GP*AP*CP*TP*GP*CP*CP*GP*GP*TP*AP*AP*C)-3')

Chain K:  48% 39% 13%



- Molecule 3: DNA (5'-D(*GP*TP*TP*AP*CP*CP*GP*GP*CP*AP*GP*TP*CP*TP*GP*CP*TP*TP*GP*TP*AP*AP*A)-3')

Chain J:  39% 61%



- Molecule 3: DNA (5'-D(*GP*TP*TP*AP*CP*CP*GP*GP*CP*AP*GP*TP*CP*TP*GP*CP*TP*TP*GP*TP*AP*AP*A)-3')

Chain L:  52% 39% 9%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.04Å 80.04Å 186.66Å 90.00° 90.07° 90.00°	Depositor
Resolution (Å)	28.50 – 3.00 28.50 – 3.00	Depositor EDS
% Data completeness (in resolution range)	94.4 (28.50-3.00) 94.1 (28.50-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 3.00Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.202 , 0.247 0.202 , 0.247	Depositor DCC
R_{free} test set	4556 reflections (9.89%)	wwPDB-VP
Wilson B-factor (Å ²)	69.2	Xtriage
Anisotropy	0.670	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 27.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l 0.000 for -k,-h,-l 0.419 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13639	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.91 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2342e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	A	0.53	0/1509	0.69	0/2046
1	B	0.51	0/1509	0.68	0/2046
1	C	0.47	0/1498	0.71	2/2032 (0.1%)
1	D	0.50	0/1498	0.68	1/2032 (0.0%)
1	E	0.51	0/1509	0.68	0/2046
1	F	0.54	0/1509	0.72	2/2046 (0.1%)
1	G	0.48	0/1509	0.68	0/2046
1	H	0.52	0/1498	0.69	0/2032
2	I	1.10	1/462 (0.2%)	1.06	2/710 (0.3%)
2	K	1.12	1/462 (0.2%)	1.06	0/710
3	J	1.08	1/525 (0.2%)	1.21	1/809 (0.1%)
3	L	1.19	2/525 (0.4%)	1.25	3/809 (0.4%)
All	All	0.63	5/14013 (0.0%)	0.78	11/19364 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	9	DC	C3'-O3'	-7.82	1.33	1.44
2	I	13	DC	C3'-O3'	-7.01	1.34	1.44
2	K	15	DG	C3'-O3'	-6.27	1.35	1.44
3	J	11	DG	C3'-O3'	-6.16	1.35	1.44
3	L	20	DT	C1'-N1	5.22	1.56	1.49

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	21	DA	O4'-C1'-N9	-7.66	102.64	108.00
3	L	19	DG	O4'-C1'-N9	7.53	113.27	108.00
3	J	8	DG	O4'-C1'-N9	5.83	112.08	108.00
2	I	17	DC	O5'-P-OP2	-5.82	100.47	105.70
1	C	115	LEU	CB-CG-CD2	-5.79	101.16	111.00
1	F	112	LEU	CA-CB-CG	-5.43	102.80	115.30
3	L	14	DT	N3-C4-O4	5.42	123.15	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	29	LEU	CA-CB-CG	-5.20	103.33	115.30
1	C	106	ASP	CB-CG-OD1	5.11	122.90	118.30
2	I	14	DT	N3-C4-O4	5.10	122.96	119.90
1	F	121	LEU	C-N-CA	-5.07	111.65	122.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1489	0	1514	27	0
1	B	1489	0	1514	18	0
1	C	1478	0	1501	27	0
1	D	1478	0	1501	31	0
1	E	1489	0	1514	21	0
1	F	1489	0	1514	25	0
1	G	1489	0	1514	29	0
1	H	1478	0	1501	16	0
2	I	411	0	223	7	0
2	K	411	0	223	6	0
3	J	469	0	262	9	0
3	L	469	0	262	6	0
All	All	13639	0	13043	191	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 7.

All (191) 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)
1:E:131:GLN:HG2	1:E:135:LEU:HD23	1.65	0.78
1:B:74:MET:SD	1:B:137:MET:HE2	2.26	0.75
1:F:131:GLN:NE2	1:F:139:GLU:OE2	2.21	0.73
1:A:162:VAL:HG13	1:D:166:ALA:HB1	1.73	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:27:TRP:CD1	1:G:32:TYR:HA	2.24	0.71
1:C:48:ARG:NH1	2:K:19:DG:N7	2.38	0.71
1:E:127:ARG:NH2	1:E:128:ASP:OD1	2.24	0.70
1:H:48:ARG:NH1	3:J:15:DG:N7	2.40	0.69
1:B:131:GLN:HG2	1:B:135:LEU:HD23	1.75	0.69
1:D:27:TRP:CD1	1:D:32:TYR:HA	2.28	0.69
1:F:7:THR:HG23	1:F:10:GLU:H	1.58	0.68
1:F:162:VAL:HG13	1:G:166:ALA:HB1	1.75	0.68
1:B:182:ARG:HG3	1:B:185:ARG:NH2	2.10	0.67
1:A:166:ALA:HB1	1:D:162:VAL:HG13	1.76	0.66
1:F:6:ARG:HH11	3:J:19:DG:H5'	1.61	0.64
1:A:7:THR:HG23	1:A:10:GLU:H	1.62	0.64
1:B:162:VAL:HG13	1:C:166:ALA:HB1	1.79	0.64
1:E:166:ALA:HB1	1:H:162:VAL:HG13	1.79	0.64
1:H:27:TRP:CD1	1:H:32:TYR:HA	2.35	0.62
1:F:8:GLN:HE22	1:F:11:ARG:NH2	1.97	0.62
1:D:98:ASP:HA	1:D:101:LEU:HD12	1.82	0.61
1:F:6:ARG:NH1	3:J:19:DG:H5'	2.15	0.61
2:K:17:DC:H2''	2:K:18:DG:C8	2.36	0.61
1:A:198:MET:SD	1:D:194:LEU:HD12	2.42	0.60
1:A:67:GLU:OE2	1:A:132:ARG:NH1	2.22	0.60
1:F:166:ALA:HB1	1:G:162:VAL:HG13	1.83	0.59
1:C:23:ALA:O	1:C:27:TRP:HB2	2.04	0.57
1:F:16:ARG:NH1	1:F:64:ASP:OD2	2.37	0.57
3:L:6:DC:H2''	3:L:7:DG:C8	2.39	0.57
1:B:119:VAL:HG21	1:C:119:VAL:HG21	1.86	0.57
1:A:153:ARG:NH2	1:E:179:ASP:OD1	2.37	0.57
1:B:23:ALA:O	1:B:27:TRP:HB2	2.05	0.57
1:E:8:GLN:OE1	1:E:11:ARG:NH1	2.37	0.56
1:C:27:TRP:CD1	1:C:32:TYR:HA	2.39	0.56
1:C:24:ARG:NE	1:C:108:GLU:OE2	2.39	0.56
1:D:163:LEU:HD11	1:D:198:MET:HE3	1.88	0.55
1:H:12:SER:OG	2:I:4:DA:H5''	2.07	0.55
1:A:188:ARG:HH21	1:A:192:ARG:NH1	2.04	0.55
1:F:8:GLN:HE22	1:F:11:ARG:HH21	1.54	0.54
1:F:101:LEU:C	1:F:184:ARG:HH12	2.11	0.54
1:H:24:ARG:NE	1:H:108:GLU:OE2	2.40	0.54
1:G:62:PHE:CE2	1:G:117:ALA:HA	2.43	0.53
1:C:70:GLU:HG2	1:C:133:TYR:CG	2.42	0.53
1:A:7:THR:HG22	1:A:10:GLU:HB3	1.91	0.53
1:F:131:GLN:NE2	1:F:139:GLU:CD	2.61	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:159:LEU:HD21	1:D:198:MET:CE	2.39	0.53
1:D:62:PHE:HE2	1:D:117:ALA:HA	1.73	0.53
1:D:159:LEU:HD21	1:D:198:MET:HE2	1.90	0.52
1:G:163:LEU:HD11	1:G:198:MET:SD	2.50	0.52
1:F:194:LEU:HD21	1:G:194:LEU:HD21	1.91	0.52
1:A:13:ALA:O	1:A:17:GLU:HG2	2.09	0.52
1:C:23:ALA:HB1	1:C:27:TRP:CE3	2.45	0.52
1:H:23:ALA:O	1:H:27:TRP:HB2	2.10	0.52
1:B:48:ARG:NH1	3:L:11:DG:N7	2.58	0.52
1:B:16:ARG:NH1	1:B:64:ASP:OD2	2.42	0.52
1:B:37:THR:OG1	1:B:48:ARG:NH2	2.43	0.52
1:C:182:ARG:HG3	1:C:185:ARG:NH1	2.25	0.52
1:D:19:LEU:HD21	1:D:51:MET:HA	1.93	0.51
1:D:52:TYR:OH	3:L:15:DG:OP2	2.26	0.51
1:B:27:TRP:CD1	1:B:32:TYR:HA	2.46	0.51
1:C:94:ARG:HD3	1:C:192:ARG:NH2	2.25	0.51
3:J:9:DC:H2"	3:J:10:DA:C8	2.46	0.51
1:A:194:LEU:HD21	1:D:194:LEU:HD21	1.93	0.50
1:D:62:PHE:CE2	1:D:117:ALA:HA	2.46	0.50
1:G:48:ARG:NH1	2:I:19:DG:N7	2.55	0.50
1:A:57:ASP:OD1	1:A:57:ASP:N	2.40	0.50
3:J:22:DA:H2"	3:J:23:DA:H5"	1.94	0.50
1:B:166:ALA:HB1	1:C:162:VAL:HG13	1.92	0.50
1:G:11:ARG:O	1:G:15:THR:HG23	2.12	0.50
1:D:163:LEU:HD11	1:D:198:MET:CE	2.42	0.50
1:F:23:ALA:O	1:F:27:TRP:HB2	2.12	0.50
1:G:6:ARG:O	1:G:11:ARG:NH1	2.44	0.50
1:G:19:LEU:HD12	1:G:44:ALA:CB	2.42	0.50
2:I:13:DC:H2"	2:I:14:DT:H72	1.94	0.49
1:B:8:GLN:HG2	1:B:11:ARG:HH21	1.76	0.49
1:E:198:MET:SD	1:H:194:LEU:HD12	2.54	0.48
1:E:68:VAL:O	1:E:71:GLN:HG2	2.13	0.48
1:B:12:SER:OG	2:K:8:DG:OP1	2.29	0.48
1:C:24:ARG:NH1	1:C:68:VAL:HG12	2.28	0.48
1:E:23:ALA:O	1:E:27:TRP:HB2	2.13	0.48
1:E:27:TRP:CD1	1:E:32:TYR:HA	2.48	0.48
1:F:68:VAL:O	1:F:71:GLN:HG2	2.14	0.47
1:E:77:MET:HG2	1:E:103:VAL:HG21	1.96	0.47
2:K:9:DC:H2"	2:K:10:DA:C8	2.49	0.47
1:G:67:GLU:OE2	1:G:132:ARG:NH1	2.31	0.47
1:A:23:ALA:O	1:A:27:TRP:HB2	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:GLN:HE22	1:D:193:ARG:HD2	1.80	0.47
1:G:167:LEU:HA	1:G:167:LEU:HD23	1.67	0.46
1:H:23:ALA:HB1	1:H:27:TRP:CE3	2.51	0.46
1:A:68:VAL:O	1:A:71:GLN:HG2	2.15	0.46
1:H:70:GLU:HG2	1:H:133:TYR:CB	2.46	0.46
1:A:144:GLU:OE2	1:A:147:ARG:NH1	2.49	0.46
1:H:67:GLU:CD	1:H:132:ARG:HH22	2.19	0.46
1:C:46:VAL:HG12	1:C:47:THR:H	1.80	0.46
1:F:27:TRP:CD1	1:F:32:TYR:HA	2.51	0.46
1:E:162:VAL:HG13	1:H:166:ALA:HB1	1.98	0.46
1:G:46:VAL:HG12	1:G:47:THR:H	1.81	0.45
1:A:32:TYR:CE1	1:A:58:LYS:HG2	2.51	0.45
1:E:7:THR:HG22	1:E:10:GLU:HG3	1.97	0.45
1:B:89:PRO:HB3	1:B:144:GLU:HG3	1.99	0.45
1:H:70:GLU:HG2	1:H:133:TYR:CG	2.52	0.45
1:F:57:ASP:N	1:F:57:ASP:OD1	2.48	0.45
1:E:12:SER:OG	3:J:4:DA:OP1	2.30	0.45
1:A:94:ARG:NH2	1:A:199:LEU:HD12	2.32	0.45
1:D:32:TYR:CE1	1:D:58:LYS:HG2	2.52	0.45
1:G:62:PHE:HE2	1:G:117:ALA:HA	1.81	0.45
1:C:62:PHE:CE2	1:C:117:ALA:HA	2.51	0.44
1:F:8:GLN:NE2	1:F:11:ARG:HH21	2.14	0.44
2:I:4:DA:C2	2:I:5:DC:C2	3.05	0.44
1:C:7:THR:HB	1:C:10:GLU:HB3	1.99	0.44
1:G:32:TYR:CE1	1:G:58:LYS:HG2	2.53	0.44
3:J:6:DC:H2''	3:J:7:DG:C8	2.53	0.44
1:B:8:GLN:HG2	1:B:11:ARG:NH2	2.33	0.44
1:D:46:VAL:HG12	1:D:47:THR:H	1.83	0.44
3:J:18:DT:H2''	3:J:19:DG:O4'	2.18	0.44
1:E:7:THR:HG23	1:E:10:GLU:H	1.83	0.44
1:A:188:ARG:HH21	1:A:192:ARG:HH12	1.65	0.44
1:E:94:ARG:HD3	1:E:192:ARG:NH1	2.32	0.44
1:C:62:PHE:HE2	1:C:117:ALA:HA	1.83	0.43
1:D:195:ILE:HA	1:D:195:ILE:HD13	1.88	0.43
1:G:192:ARG:HG3	1:G:193:ARG:N	2.33	0.43
1:C:114:LEU:HD23	1:C:114:LEU:HA	1.66	0.43
1:C:163:LEU:O	1:C:167:LEU:HG	2.18	0.43
1:D:12:SER:OG	1:D:54:GLN:NE2	2.46	0.43
1:H:32:TYR:CE1	1:H:58:LYS:HG2	2.53	0.43
1:F:19:LEU:HD12	1:F:44:ALA:CB	2.49	0.43
1:H:57:ASP:OD1	1:H:57:ASP:N	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:48:ARG:NH1	3:L:15:DG:N7	2.63	0.43
2:K:13:DC:H2"	2:K:14:DT:H72	2.00	0.43
1:E:19:LEU:HD12	1:E:44:ALA:CB	2.49	0.43
1:G:8:GLN:H	1:G:8:GLN:CD	2.21	0.43
1:C:57:ASP:N	1:C:57:ASP:OD1	2.52	0.43
1:D:7:THR:HG22	1:D:10:GLU:CD	2.39	0.43
1:C:188:ARG:HH12	1:C:192:ARG:NH1	2.16	0.43
1:G:112:LEU:O	1:G:117:ALA:HB2	2.18	0.43
1:A:77:MET:HG2	1:A:103:VAL:HG21	2.01	0.43
1:A:154:GLN:NE2	1:D:193:ARG:HD2	2.34	0.43
1:E:46:VAL:HG12	1:E:47:THR:H	1.83	0.42
1:B:77:MET:HG2	1:B:103:VAL:HG21	2.02	0.42
1:D:182:ARG:NH1	1:E:178:ASP:OD1	2.52	0.42
1:G:6:ARG:HG2	1:G:6:ARG:HH21	1.84	0.42
1:A:112:LEU:HA	1:A:112:LEU:HD23	1.87	0.42
1:D:7:THR:HG22	1:D:10:GLU:CG	2.49	0.42
1:F:70:GLU:HG2	1:F:133:TYR:CD2	2.54	0.42
1:G:157:ARG:HB2	1:G:158:PRO:HD3	2.02	0.42
2:I:10:DA:H2"	2:I:11:DG:C8	2.54	0.42
3:L:20:DT:H2"	3:L:21:DA:H5"	2.01	0.42
3:L:22:DA:H2"	3:L:23:DA:H5"	2.02	0.42
1:C:19:LEU:HD12	1:C:44:ALA:CB	2.49	0.42
1:D:130:ALA:O	1:D:135:LEU:HB3	2.19	0.42
1:G:54:GLN:HA	1:G:54:GLN:OE1	2.20	0.42
1:A:46:VAL:HG12	1:A:50:ALA:HB3	2.02	0.42
1:C:37:THR:OG1	1:C:38:PRO:HD3	2.20	0.42
1:C:167:LEU:HD23	1:C:167:LEU:HA	1.61	0.42
2:I:18:DG:H1'	2:I:19:DG:H5'	2.02	0.42
1:F:169:GLU:HG3	1:G:165:GLY:CA	2.50	0.42
1:D:67:GLU:CD	1:D:132:ARG:HH22	2.23	0.42
1:E:77:MET:HE3	1:E:99:ALA:HB3	2.01	0.42
1:A:38:PRO:HG3	1:A:48:ARG:HD2	2.01	0.41
1:G:8:GLN:HG2	1:G:9:GLU:N	2.35	0.41
1:B:117:ALA:HB3	1:B:118:PRO:HD3	2.02	0.41
1:D:159:LEU:HD11	1:D:198:MET:HE3	2.02	0.41
1:D:46:VAL:HG12	1:D:50:ALA:HB3	2.03	0.41
1:F:46:VAL:HG12	1:F:47:THR:H	1.85	0.41
2:I:13:DC:H2"	2:I:14:DT:C7	2.49	0.41
1:A:141:LEU:HA	1:A:141:LEU:HD23	1.82	0.41
1:H:163:LEU:O	1:H:167:LEU:HG	2.19	0.41
1:A:32:TYR:HE1	1:A:58:LYS:HG2	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:LEU:HA	1:C:141:LEU:HD23	1.85	0.41
1:D:7:THR:HG22	1:D:10:GLU:HG3	2.03	0.41
1:C:117:ALA:HB3	1:C:118:PRO:HD3	2.03	0.41
3:J:13:DC:H2'	3:J:14:DT:H72	2.02	0.41
1:B:182:ARG:HG3	1:B:185:ARG:HH22	1.84	0.41
1:F:165:GLY:CA	1:G:169:GLU:HG3	2.50	0.41
1:E:167:LEU:O	1:E:170:ALA:HB3	2.21	0.41
1:F:169:GLU:HG3	1:G:165:GLY:HA2	2.03	0.41
1:G:189:GLN:O	1:G:192:ARG:HG2	2.20	0.41
1:A:101:LEU:HD23	1:A:101:LEU:HA	1.88	0.41
1:F:38:PRO:HG3	1:F:48:ARG:HD2	2.02	0.41
1:G:27:TRP:HB3	1:G:112:LEU:HD21	2.03	0.41
1:A:27:TRP:CD1	1:A:32:TYR:HA	2.55	0.40
1:D:77:MET:HG2	1:D:103:VAL:HG21	2.03	0.40
2:K:13:DC:H2''	2:K:14:DT:C7	2.51	0.40
1:E:195:ILE:HA	1:E:195:ILE:HD13	1.98	0.40
1:G:23:ALA:O	1:G:27:TRP:HB2	2.20	0.40
1:C:32:TYR:CE1	1:C:58:LYS:HG2	2.57	0.40
1:C:70:GLU:HG2	1:C:133:TYR:CD2	2.57	0.40
1:D:54:GLN:HA	1:D:54:GLN:OE1	2.20	0.40
1:F:130:ALA:O	1:F:135:LEU:HB3	2.21	0.40
1:G:182:ARG:HG3	1:G:185:ARG:NH1	2.36	0.40
1:H:188:ARG:O	1:H:192:ARG:HG2	2.22	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	A	193/214 (90%)	189 (98%)	4 (2%)	0	100	100
1	B	193/214 (90%)	187 (97%)	6 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	192/214 (90%)	188 (98%)	4 (2%)	0	100	100
1	D	192/214 (90%)	188 (98%)	4 (2%)	0	100	100
1	E	193/214 (90%)	188 (97%)	5 (3%)	0	100	100
1	F	193/214 (90%)	187 (97%)	6 (3%)	0	100	100
1	G	193/214 (90%)	189 (98%)	4 (2%)	0	100	100
1	H	192/214 (90%)	188 (98%)	4 (2%)	0	100	100
All	All	1541/1712 (90%)	1504 (98%)	37 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	
1	A	146/161 (91%)	146 (100%)	0	100	100
1	B	146/161 (91%)	146 (100%)	0	100	100
1	C	145/161 (90%)	145 (100%)	0	100	100
1	D	145/161 (90%)	145 (100%)	0	100	100
1	E	146/161 (91%)	146 (100%)	0	100	100
1	F	146/161 (91%)	146 (100%)	0	100	100
1	G	146/161 (91%)	146 (100%)	0	100	100
1	H	145/161 (90%)	143 (99%)	2 (1%)	67	88
All	All	1165/1288 (90%)	1163 (100%)	2 (0%)	93	98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	88	THR
1	H	198	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such

sidechains are listed below:

Mol	Chain	Res	Type
1	D	54	GLN
1	E	161	GLN
1	F	8	GLN
1	G	161	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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	195/214 (91%)	-0.48	0 100 100	43, 62, 84, 110	0
1	B	195/214 (91%)	-0.52	0 100 100	44, 64, 89, 112	0
1	C	194/214 (90%)	-0.51	0 100 100	45, 65, 93, 135	0
1	D	194/214 (90%)	-0.49	0 100 100	46, 68, 93, 130	0
1	E	195/214 (91%)	-0.50	0 100 100	42, 63, 87, 108	0
1	F	195/214 (91%)	-0.48	0 100 100	45, 63, 86, 120	0
1	G	195/214 (91%)	-0.47	0 100 100	46, 71, 100, 175	0
1	H	194/214 (90%)	-0.52	0 100 100	44, 64, 91, 136	0
2	I	20/23 (86%)	-0.69	0 100 100	70, 88, 166, 171	0
2	K	20/23 (86%)	-0.63	0 100 100	71, 85, 164, 171	0
3	J	23/23 (100%)	-0.43	0 100 100	68, 89, 179, 191	0
3	L	23/23 (100%)	-0.43	0 100 100	67, 92, 180, 191	0
All	All	1643/1804 (91%)	-0.50	0 100 100	42, 65, 99, 191	0

There are no RSRZ outliers to report.

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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.