



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 01:50 PM GMT

PDB ID : 1C7Y  
Title : E.COLI RUVA-HOLLIDAY JUNCTION COMPLEX  
Authors : Ariyoshi, M.; Nishino, T.; Iwasaki, H.; Shinagawa, H.; Morikawa, K.  
Deposited on : 2000-04-03  
Resolution : 3.10 Å(reported)

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

---

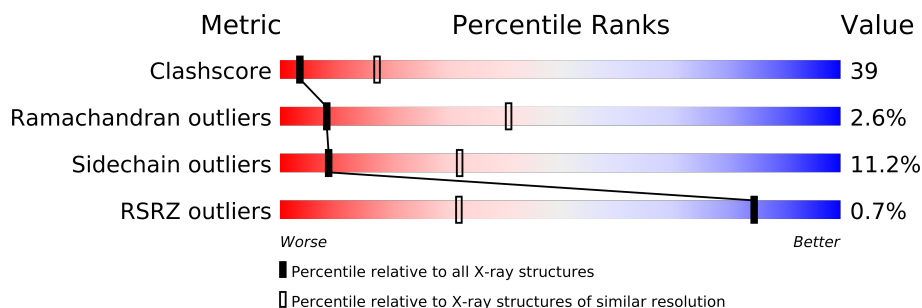
The following versions of software and data (see [references](#)) were used in the production of this report:

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

# 1 Overall quality at a glance

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)
RSRZ outliers	66119	1008 (3.18-3.02)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	B	13	
2	C	12	
3	D	13	
4	E	12	
5	F	13	
6	G	12	
7	H	13	
8	I	12	
9	A	203	

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 3565 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a DNA chain called DNA (5'-D(P\*DAP\*DAP\*DGP\*DTP\*DTP\*DGP\*DGP\*DGP\*DAP\*DTP\*DTP\*DGP\*DT)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	13	Total	C	N	O	P	0	13	0
			270	130	50	78	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	12	Total	C	N	O	P	0	12	0
			248	118	44	74	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	13	Total	C	N	O	P	0	13	0
			262	126	51	73	12			

- Molecule 4 is a DNA chain called DNA (5'-D(P\*DGP\*DGP\*DTP\*DTP\*DAP\*DGP\*DGP\*DGP\*DTP\*DGP\*DAP\*DA)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	12	Total	C	N	O	P	0	12	0
			255	120	51	72	12			

- Molecule 5 is a DNA chain called DNA (5'-D(P\*DTP\*DTP\*DCP\*DAP\*DCP\*DCP\*DCP\*DTP\*DAP\*DAP\*DCP\*DCP\*DA)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	13	Total	C	N	O	P	0	13	0
			255	124	44	75	12			

- Molecule 6 is a DNA chain called DNA (5'-D(P\*DGP\*DAP\*DCP\*DAP\*DCP\*DAP\*DCP\*DAP\*DTP\*DTP\*DCP\*DG)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	12	Total	C	N	O	P	0	12	0
			244	116	46	70	12			

- Molecule 7 is a DNA chain called DNA (5'-D(P\*DCP\*DGP\*DAP\*DAP\*DTP\*DGP\*DTP\*DGP\*DTP\*DGP\*DTP\*DCP\*DT)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	13	Total	C	N	O	P	0	13	0
			265	128	46	79	12			

- Molecule 8 is a DNA chain called DNA (5'-D(P\*DCP\*DAP\*DAP\*DTP\*DCP\*DCP\*DCP\*DAP\*DAP\*DCP\*DTP\*DT)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	12	Total	C	N	O	P	0	12	0
			239	115	41	71	12			

- Molecule 9 is a protein called HOLLIDAY JUNCTION DNA HELICASE RUVA.

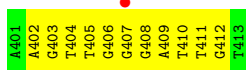
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	A	199	Total	C	N	O	S	0	0	0
			1527	974	262	284	7			

### 3 Residue-property plots

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

- Molecule 1: DNA (5'-D(P\*DAP\*DAP\*DGP\*DTP\*DTP\*DGP\*DGP\*DGP\*DAP\*DTP\*DTP\*DGP\*DT)-3')

Chain B: 



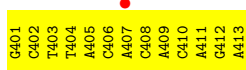
- Molecule 2: DNA (5'-D(P\*DCP\*DTP\*DGP\*DTP\*DGP\*DTP\*DGP\*DTP\*DAP\*DAP\*DGP\*DC)-3')

Chain C: 



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

Chain D: 



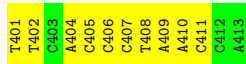
- Molecule 4: DNA (5'-D(P\*DGP\*DGP\*DTP\*DTP\*DAP\*DGP\*DGP\*DGP\*DTP\*DGP\*DAP\*DA)-3')

Chain E: 



- Molecule 5: DNA (5'-D(P\*DTP\*DTP\*DCP\*DAP\*DCP\*DCP\*DCP\*DTP\*DAP\*DAP\*DCP\*DCP\*DA)-3')

Chain F: 



- Molecule 6: DNA (5'-D(P\*DGP\*DAP\*DCP\*DAP\*DCP\*DAP\*DCP\*DAP\*DTP\*DTP\*DCP\*DG)-3')

Chain G: 

G501	A502	C503	A504	C505	A506	C507	A508	T509	T510	C511	G512
------	------	------	------	------	------	------	------	------	------	------	------

- Molecule 7: DNA (5'-D(P\*DCP\*DGP\*DAP\*DAP\*DTP\*DGP\*DTP\*DGP\*DTP\*DGP\*DTP\*DCP\*DT)-3')

Chain H: 

C401	G402	A403	A404	T405	G406	T407	G408	T409	G410	T411	C412	T413
------	------	------	------	------	------	------	------	------	------	------	------	------

- Molecule 8: DNA (5'-D(P\*DCP\*DAP\*DAP\*DTP\*DCP\*DCP\*DCP\*DAP\*DAP\*DCP\*DTP\*DT)-3')

Chain I: 

C501	A502	A503	T504	C505	C506	C507	A508	A509	C510	T511	T512
------	------	------	------	------	------	------	------	------	------	------	------

- Molecule 9: HOLLIDAY JUNCTION DNA HELICASE RUVA

Chain A: 

R1	R6	I10	E11	K12	Q13	V17	L18	K30	T33	Y36	E37	I46	V47	F48	T49	H50	V53	R54	E55	D56	A57	R58	L59	L60	V61	G62	F63	N64	N65	R66	Q67	E68	R69	T70	L71	F72	K73	E74	L75	I76	N79	G80	V81	G82	P83	X84	L85	I89							
M93	S94	A95	Q96	Q97	F98	V99	V102	E103	R104	V107	G108	A109	L110	V111	K112	I116	G117	K118	K119	T120	A121	E122	R123	L124	I125	V126	E127	M128	K129	D130	R131	F132	K133	G134	L135	H136	L139	F140	T141	F142	A143	A144	D145	L146	V147	L148	T149	S150	P150	ALA	SER	PRO	A155	T156	D157
D158	A159	E160	Q161	E162	A163	V164	A165	K173	E176	A177	S178	R179	M180	V181	S182	K183	T184	A185	R186	P187	D188	S191	E192	T193	L194	E197	N198	L199	R200	L203																									

## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	158.65Å 158.65Å 158.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.80 – 3.10 50.17 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.80-3.10) 99.9 (50.17-3.00)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	9.44 (at 3.01Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, $R_{free}$	0.249 , 0.279 0.247 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	64.6	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 47.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 7133 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	3565	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	B	0.28	0/303	0.62	0/468
2	C	0.33	0/277	0.66	0/426
3	D	0.29	0/294	0.64	0/451
4	E	0.31	0/287	0.63	0/443
5	F	0.32	0/284	0.66	0/434
6	G	0.38	0/273	0.76	0/418
7	H	0.35	0/296	0.75	0/456
8	I	0.33	0/266	0.66	0/406
9	A	0.85	5/1549 (0.3%)	1.02	7/2088 (0.3%)
All	All	0.60	5/3829 (0.1%)	0.82	7/5590 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
9	A	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	116	ILE	C-N	15.58	1.61	1.33
9	A	117	GLY	CA-C	7.73	1.64	1.51
9	A	53	VAL	C-N	-5.83	1.20	1.34
9	A	118	LYS	N-CA	5.34	1.57	1.46
9	A	155	ALA	CA-CB	5.17	1.63	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	116	ILE	CB-CA-C	-14.01	83.58	111.60
9	A	134	GLY	N-CA-C	-11.92	83.31	113.10

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	53	VAL	C-N-CA	7.16	139.59	121.70
9	A	116	ILE	C-N-CA	-7.14	107.30	122.30
9	A	54	ARG	CB-CA-C	6.26	122.92	110.40
9	A	53	VAL	O-C-N	-5.32	114.19	122.70
9	A	149	THR	N-CA-C	5.04	124.61	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	A	132	PHE	Mainchain

## 5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	270	0	124	25	0
2	C	248	0	118	28	0
3	D	262	0	125	34	0
4	E	255	0	114	32	0
5	F	255	0	127	17	0
6	G	244	0	116	21	0
7	H	265	0	126	24	0
8	I	239	0	120	28	0
9	A	1527	0	1579	101	3
All	All	3565	0	2549	240	3

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 39.

All (240) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:403[A]:DG:N1	2:C:510[A]:DA:C2	1.81	1.48
1:B:403[A]:DG:N1	2:C:510[A]:DA:H2	0.93	1.40
7:H:410[D]:DG:N1	8:I:503[D]:DA:N1	1.72	1.36

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:H:410[D]:DG:N2	8:I:503[D]:DA:H2	1.30	1.26
1:B:403[A]:DG:O6	2:C:510[A]:DA:N1	1.66	1.23
7:H:410[D]:DG:N1	8:I:503[D]:DA:C2	2.05	1.21
5:F:409[C]:DA:C2	6:G:504[C]:DA:N1	2.09	1.21
3:D:412[B]:DG:O6	4:E:501[B]:DG:O6	1.60	1.16
1:B:402[A]:DA:N6	2:C:511[A]:DG:N1	1.91	1.11
3:D:413[B]:DA:N3	4:E:501[B]:DG:N2	1.96	1.11
9:A:116:ILE:O	9:A:116:ILE:HG22	1.33	1.10
7:H:410[D]:DG:N2	8:I:503[D]:DA:C2	2.22	1.08
9:A:116:ILE:O	9:A:116:ILE:CG2	1.91	1.07
7:H:410[D]:DG:C2	8:I:503[D]:DA:H2	1.73	1.06
5:F:409[C]:DA:H2	6:G:504[C]:DA:N1	1.51	1.01
1:B:403[A]:DG:C6	2:C:510[A]:DA:C2	2.48	1.00
3:D:413[B]:DA:C2	4:E:501[B]:DG:N1	2.32	0.97
7:H:404[D]:DA:H61	8:I:509[D]:DA:N6	1.63	0.97
9:A:6:ARG:HG3	9:A:46:ILE:HG12	1.44	0.97
7:H:410[D]:DG:C2	8:I:503[D]:DA:C2	2.52	0.96
3:D:411[B]:DA:C2	4:E:502[B]:DG:N1	2.32	0.96
9:A:176:GLU:HG3	9:A:179:ARG:HH11	1.30	0.95
1:B:403[A]:DG:C6	2:C:510[A]:DA:N1	2.36	0.94
3:D:413[B]:DA:C2	4:E:501[B]:DG:C2	2.57	0.93
5:F:409[C]:DA:N1	6:G:504[C]:DA:N1	2.18	0.91
7:H:404[D]:DA:H61	8:I:509[D]:DA:H61	1.17	0.91
3:D:413[B]:DA:N3	4:E:501[B]:DG:C2	2.40	0.90
3:D:412[B]:DG:C2	4:E:502[B]:DG:N2	2.39	0.90
9:A:67:GLN:HE21	9:A:67:GLN:H	1.20	0.88
3:D:407[B]:DA:N6	4:E:506[B]:DG:O6	2.07	0.87
4:E:501[B]:DG:P	4:E:501[B]:DG:H3'	2.16	0.86
7:H:410[D]:DG:C6	8:I:503[D]:DA:N1	2.44	0.85
9:A:65:ASN:HB2	9:A:68:GLU:HG3	1.57	0.85
7:H:404[D]:DA:N6	8:I:509[D]:DA:H61	1.76	0.84
7:H:408[D]:DG:H1'	7:H:409[D]:DT:H5'	1.60	0.84
9:A:94:SER:OG	9:A:97:GLN:HG3	1.79	0.82
8:I:505[D]:DC:P	9:A:123:ARG:HH12	2.03	0.82
3:D:411[B]:DA:H2	4:E:502[B]:DG:N1	1.72	0.82
1:B:402[A]:DA:N6	2:C:511[A]:DG:C6	2.48	0.82
5:F:409[C]:DA:H2	6:G:504[C]:DA:C2	1.98	0.81
9:A:67:GLN:NE2	9:A:67:GLN:H	1.80	0.79
3:D:412[B]:DG:C6	4:E:501[B]:DG:O6	2.34	0.79
4:E:505[B]:DA:OP1	9:A:123:ARG:NH1	2.14	0.78
9:A:181:VAL:O	9:A:184:ILE:HG12	1.83	0.78
9:A:176:GLU:HG3	9:A:179:ARG:NH1	1.99	0.78

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:A:200:ARG:HB3	9:A:200:ARG:HH11	1.49	0.77
6:G:506[C]:DA:OP1	9:A:120:THR:HG23	1.85	0.77
9:A:81:VAL:HA	9:A:85:LEU:HD12	1.68	0.76
6:G:504[C]:DA:H1'	6:G:505[C]:DC:H5''	1.68	0.76
9:A:79:ASN:OD1	9:A:79:ASN:C	2.22	0.76
2:C:505[A]:DG:OP1	9:A:123:ARG:NH1	2.17	0.75
2:C:505[A]:DG:H2'	2:C:506[A]:DT:H71	1.68	0.75
5:F:409[C]:DA:N1	6:G:504[C]:DA:N6	2.34	0.75
3:D:405[B]:DA:H2''	3:D:406[B]:DC:H5'	1.70	0.74
1:B:409[A]:DA:N1	2:C:504[A]:DT:N3	2.35	0.74
4:E:501[B]:DG:H2''	4:E:502[B]:DG:C8	2.22	0.73
9:A:102:VAL:HA	9:A:125:ILE:HG22	1.69	0.73
1:B:405[A]:DT:H1'	1:B:406[A]:DG:H5''	1.71	0.72
3:D:403[B]:DT:N3	4:E:510[B]:DG:N1	2.36	0.72
4:E:504[B]:DT:H2''	4:E:505[B]:DA:H5''	1.71	0.72
8:I:505[D]:DC:OP1	9:A:123:ARG:NH1	2.21	0.71
3:D:412[B]:DG:N2	4:E:502[B]:DG:C2	2.59	0.71
9:A:145:ASP:O	9:A:149:THR:HB	1.90	0.71
1:B:403[A]:DG:C2	2:C:510[A]:DA:H2	2.02	0.70
5:F:409[C]:DA:N1	6:G:504[C]:DA:C6	2.61	0.68
3:D:405[B]:DA:H2''	3:D:406[B]:DC:C5'	2.24	0.68
3:D:403[B]:DT:O2	4:E:510[B]:DG:N2	2.26	0.68
3:D:405[B]:DA:H1'	3:D:406[B]:DC:H5''	1.76	0.67
7:H:405[D]:DT:H1'	7:H:406[D]:DG:H5''	1.76	0.67
2:C:511[A]:DG:H2''	2:C:512[A]:DC:H5'	1.76	0.67
7:H:404[D]:DA:N6	8:I:509[D]:DA:N6	2.38	0.67
2:C:504[A]:DT:H2''	2:C:505[A]:DG:H5''	1.77	0.66
9:A:67:GLN:N	9:A:67:GLN:HE21	1.92	0.66
6:G:511[C]:DC:H2''	6:G:512[C]:DG:H5'	1.77	0.66
5:F:401[C]:DT:H2'	5:F:402[C]:DT:H71	1.78	0.66
6:G:505[C]:DC:OP1	9:A:123:ARG:NH1	2.29	0.66
9:A:122:GLU:HA	9:A:125:ILE:HD11	1.78	0.66
6:G:501[C]:DG:H3'	6:G:501[C]:DG:P	2.35	0.65
4:E:506[B]:DG:OP1	9:A:120:THR:HG23	1.95	0.65
4:E:511[B]:DA:H2''	4:E:512[B]:DA:H5'	1.79	0.65
9:A:99:VAL:O	9:A:102:VAL:HG22	1.96	0.65
3:D:412[B]:DG:O6	4:E:501[B]:DG:C6	2.43	0.64
9:A:37:GLU:HB2	9:A:64:ASN:ND2	2.12	0.64
9:A:99:VAL:HA	9:A:132:PHE:HE1	1.61	0.64
8:I:506[D]:DC:OP1	9:A:120:THR:HG23	1.96	0.64
9:A:95:ALA:O	9:A:99:VAL:HG23	1.97	0.64
3:D:407[B]:DA:N6	4:E:506[B]:DG:C6	2.65	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:G:501[C]:DG:H2''	6:G:502[C]:DA:C8	2.32	0.63
9:A:99:VAL:HA	9:A:132:PHE:CE1	2.33	0.63
9:A:145:ASP:HA	9:A:148:LEU:HD12	1.80	0.63
3:D:412[B]:DG:C2	4:E:502[B]:DG:C2	2.87	0.63
8:I:501[D]:DC:H2''	8:I:502[D]:DA:C8	2.33	0.63
3:D:412[B]:DG:N3	4:E:502[B]:DG:N2	2.46	0.63
3:D:410[B]:DC:H2''	3:D:411[B]:DA:C8	2.34	0.62
7:H:404[D]:DA:H2''	7:H:405[D]:DT:H71	1.81	0.62
9:A:162:GLU:O	9:A:165:ALA:HB3	1.99	0.62
7:H:404[D]:DA:N6	8:I:509[D]:DA:C6	2.67	0.61
3:D:409[B]:DA:N1	4:E:504[B]:DT:N3	2.48	0.61
9:A:79:ASN:OD1	9:A:80:GLY:N	2.33	0.61
7:H:404[D]:DA:C2'	7:H:405[D]:DT:H71	2.30	0.61
2:C:506[A]:DT:OP1	9:A:120:THR:HG23	1.99	0.61
3:D:411[B]:DA:N1	4:E:502[B]:DG:N1	2.48	0.61
2:C:505[A]:DG:P	9:A:123:ARG:HH12	2.07	0.61
8:I:511[D]:DT:H2''	8:I:512[D]:DT:H5'	1.83	0.61
7:H:408[D]:DG:H1'	7:H:409[D]:DT:C5'	2.29	0.60
3:D:403[B]:DT:O4	4:E:510[B]:DG:O6	2.19	0.60
5:F:405[C]:DC:H1'	5:F:406[C]:DC:H5''	1.83	0.60
1:B:409[A]:DA:N6	2:C:504[A]:DT:O4	2.35	0.60
9:A:139:LEU:O	9:A:139:LEU:HG	2.01	0.60
9:A:10:ILE:HB	9:A:18:LEU:HD13	1.84	0.58
7:H:410[D]:DG:H2'	7:H:411[D]:DT:H72	1.85	0.58
1:B:405[A]:DT:H2''	1:B:406[A]:DG:H5'	1.85	0.58
6:G:505[C]:DC:OP1	9:A:119:LYS:NZ	2.30	0.57
6:G:510[C]:DT:H2''	6:G:511[C]:DC:OP2	2.04	0.57
6:G:507[C]:DC:H4'	6:G:508[C]:DA:OP1	2.05	0.56
9:A:120:THR:HA	9:A:123:ARG:HD2	1.86	0.56
2:C:501[A]:DC:H5'	2:C:501[A]:DC:H6	1.70	0.56
1:B:405[A]:DT:H2''	1:B:406[A]:DG:C5'	2.36	0.56
9:A:177:ALA:HA	9:A:180:MET:HE3	1.87	0.55
9:A:146:LEU:HD21	9:A:162:GLU:HA	1.88	0.55
9:A:176:GLU:CG	9:A:179:ARG:HH11	2.12	0.55
1:B:411[A]:DT:H2''	1:B:412[A]:DG:C8	2.41	0.55
9:A:185:ALA:O	9:A:186:ARG:HG2	2.06	0.55
9:A:176:GLU:O	9:A:180:MET:HB2	2.07	0.54
6:G:504[C]:DA:H2''	6:G:505[C]:DC:OP2	2.06	0.54
6:G:505[C]:DC:H2''	6:G:506[C]:DA:H8	1.73	0.54
9:A:176:GLU:HA	9:A:179:ARG:NE	2.22	0.54
9:A:164:VAL:HG22	9:A:181:VAL:HG21	1.90	0.54
8:I:501[D]:DC:H3'	8:I:501[D]:DC:P	2.48	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:H:409[D]:DT:H2''	7:H:410[D]:DG:C8	2.43	0.53
8:I:504[D]:DT:H2''	8:I:505[D]:DC:H5''	1.90	0.53
2:C:507[A]:DG:H4'	2:C:508[A]:DT:OP1	2.08	0.53
9:A:103:GLU:OE2	9:A:133:LYS:HB2	2.08	0.53
9:A:85:LEU:O	9:A:89:ILE:HG13	2.09	0.53
8:I:501[D]:DC:H6	8:I:501[D]:DC:H5'	1.73	0.53
7:H:402[D]:DG:H2''	7:H:403[D]:DA:OP2	2.09	0.52
7:H:405[D]:DT:N3	8:I:508[D]:DA:N1	2.57	0.52
9:A:164:VAL:CG2	9:A:181:VAL:HG21	2.40	0.52
9:A:98:PHE:HZ	9:A:124:LEU:HD12	1.73	0.52
1:B:402[A]:DA:N6	2:C:511[A]:DG:O6	2.41	0.52
5:F:405[C]:DC:H2''	5:F:406[C]:DC:C5'	2.40	0.52
5:F:407[C]:DC:H1'	5:F:408[C]:DT:H5'	1.92	0.52
5:F:404[C]:DA:N6	6:G:508[C]:DA:N6	2.59	0.51
9:A:160:GLU:O	9:A:164:VAL:HG23	2.11	0.51
3:D:412[B]:DG:N2	4:E:502[B]:DG:N2	2.58	0.51
9:A:157:ASP:HB2	9:A:187:PRO:HB2	1.92	0.51
6:G:509[C]:DT:H2''	6:G:510[C]:DT:OP2	2.11	0.51
9:A:176:GLU:O	9:A:180:MET:HE2	2.11	0.50
9:A:200:ARG:HH11	9:A:200:ARG:CB	2.21	0.50
9:A:176:GLU:CG	9:A:179:ARG:NH1	2.71	0.50
9:A:182:SER:O	9:A:185:ALA:N	2.43	0.50
9:A:107:VAL:O	9:A:111:VAL:HG23	2.12	0.50
3:D:409[B]:DA:H2''	3:D:410[B]:DC:C5	2.46	0.50
5:F:410[C]:DA:H2''	5:F:411[C]:DC:C6	2.47	0.50
9:A:98:PHE:O	9:A:102:VAL:HG13	2.11	0.50
9:A:95:ALA:HB1	9:A:139:LEU:HD22	1.93	0.50
9:A:109:ALA:O	9:A:112:LYS:HG3	2.12	0.50
1:B:409[A]:DA:H2''	1:B:410[A]:DT:C6	2.47	0.50
5:F:409[C]:DA:H2''	5:F:410[C]:DA:C8	2.47	0.49
9:A:184:ILE:HD13	9:A:184:ILE:N	2.27	0.49
9:A:162:GLU:HG2	9:A:191:SER:HB2	1.94	0.49
1:B:408[A]:DG:N2	2:C:506[A]:DT:O2	2.45	0.49
1:B:412[A]:DG:N2	2:C:501[A]:DC:N3	2.60	0.49
9:A:164:VAL:HG13	9:A:177:ALA:HB1	1.95	0.49
8:I:511[D]:DT:H2''	8:I:512[D]:DT:C5'	2.43	0.49
9:A:118:LYS:O	9:A:122:GLU:HG3	2.13	0.48
4:E:505[B]:DA:P	9:A:123:ARG:HH12	2.17	0.48
9:A:164:VAL:HG13	9:A:177:ALA:CB	2.43	0.48
9:A:102:VAL:HG21	9:A:132:PHE:CD1	2.48	0.48
9:A:72:PHE:HA	9:A:75:LEU:HD12	1.96	0.48
1:B:403[A]:DG:C8	1:B:404[A]:DT:H72	2.48	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:A:50:HIS:ND1	9:A:73:LYS:HE2	2.29	0.48
3:D:404[B]:DT:H2''	3:D:405[B]:DA:C8	2.48	0.48
7:H:403[D]:DA:H2''	7:H:404[D]:DA:OP2	2.13	0.48
9:A:102:VAL:HG21	9:A:132:PHE:CE1	2.49	0.48
5:F:405[C]:DC:H2''	5:F:406[C]:DC:H5'	1.96	0.47
2:C:511[A]:DG:H2''	2:C:512[A]:DC:C5'	2.41	0.47
9:A:145:ASP:O	9:A:149:THR:CB	2.60	0.47
9:A:118:LYS:HE2	9:A:122:GLU:OE2	2.14	0.47
8:I:507[D]:DC:H4'	8:I:508[D]:DA:OP1	2.14	0.47
7:H:401[D]:DC:H2''	7:H:402[D]:DG:C8	2.49	0.47
3:D:402[B]:DC:H2''	3:D:403[B]:DT:H71	1.97	0.47
9:A:54:ARG:HB2	9:A:57:ALA:O	2.15	0.47
1:B:409[A]:DA:H2''	1:B:410[A]:DT:C5	2.50	0.47
3:D:409[B]:DA:H2''	3:D:410[B]:DC:C6	2.50	0.47
9:A:182:SER:O	9:A:183:LYS:C	2.53	0.47
9:A:37:GLU:HB2	9:A:64:ASN:HD21	1.80	0.47
9:A:93:MET:HB2	9:A:97:GLN:HB2	1.98	0.46
2:C:505[A]:DG:C2'	2:C:506[A]:DT:H71	2.43	0.46
7:H:410[D]:DG:O6	8:I:503[D]:DA:N1	2.46	0.46
9:A:144:ALA:O	9:A:147:VAL:HB	2.15	0.46
9:A:110:LEU:O	9:A:116:ILE:HG21	2.16	0.46
9:A:176:GLU:C	9:A:180:MET:HE2	2.36	0.46
9:A:179:ARG:HG3	9:A:180:MET:N	2.31	0.46
1:B:406[A]:DG:H2''	1:B:407[A]:DG:C8	2.51	0.45
1:B:410[A]:DT:C6	1:B:411[A]:DT:H72	2.51	0.45
4:E:501[B]:DG:P	4:E:501[B]:DG:C3'	2.97	0.45
9:A:157:ASP:HB2	9:A:187:PRO:CB	2.46	0.44
9:A:95:ALA:CB	9:A:139:LEU:HD22	2.48	0.44
9:A:146:LEU:HD13	9:A:161:GLN:HB2	1.98	0.44
3:D:402[B]:DC:C2'	3:D:403[B]:DT:H71	2.47	0.44
2:C:501[A]:DC:H3'	2:C:501[A]:DC:P	2.58	0.44
9:A:122:GLU:O	9:A:125:ILE:HG13	2.18	0.44
9:A:94:SER:HG	9:A:97:GLN:HG3	1.79	0.44
1:B:404[A]:DT:N3	2:C:509[A]:DA:N1	2.65	0.44
8:I:505[D]:DC:H2''	8:I:506[D]:DC:H6	1.82	0.43
6:G:505[C]:DC:H2''	6:G:506[C]:DA:C8	2.53	0.43
8:I:503[D]:DA:H2''	8:I:504[D]:DT:C5	2.54	0.43
8:I:503[D]:DA:H2''	8:I:504[D]:DT:C6	2.53	0.43
4:E:510[B]:DG:H2''	4:E:511[B]:DA:C8	2.54	0.43
2:C:501[A]:DC:H2''	2:C:502[A]:DT:C6	2.54	0.43
3:D:406[B]:DC:H2''	3:D:407[B]:DA:C8	2.54	0.43
9:A:120:THR:O	9:A:121:ALA:C	2.57	0.43

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:A:107:VAL:O	9:A:108:GLY:C	2.56	0.42
5:F:406[C]:DC:H2''	5:F:407[C]:DC:C6	2.54	0.42
9:A:112:LYS:HB3	9:A:112:LYS:HE2	1.87	0.42
9:A:73:LYS:O	9:A:76:ILE:HG12	2.19	0.42
1:B:408[A]:DG:H1'	1:B:409[A]:DA:H5'	2.01	0.42
9:A:11:GLU:OE2	9:A:13:GLN:NE2	2.52	0.42
9:A:143:ALA:HB2	9:A:158:ASP:OD2	2.19	0.42
5:F:410[C]:DA:H2''	5:F:411[C]:DC:H6	1.81	0.42
9:A:70:THR:O	9:A:74:GLU:HG2	2.18	0.42
3:D:411[B]:DA:H2	4:E:502[B]:DG:C2	2.35	0.42
9:A:177:ALA:O	9:A:181:VAL:HG23	2.19	0.42
2:C:501[A]:DC:H2'	2:C:502[A]:DT:H71	2.02	0.41
9:A:61:TYR:CE1	9:A:83:PRO:HB3	2.56	0.41
5:F:404[C]:DA:C6	6:G:508[C]:DA:N6	2.88	0.41
2:C:508[A]:DT:H2''	2:C:509[A]:DA:C8	2.55	0.41
3:D:407[B]:DA:H1'	3:D:408[B]:DC:H5'	2.02	0.41
9:A:133:LYS:CD	9:A:136:HIS:HA	2.50	0.41
9:A:30:MET:HG2	9:A:62:GLY:O	2.20	0.41
3:D:401[B]:DG:H2''	3:D:402[B]:DC:C6	2.55	0.41
9:A:33:THR:HA	9:A:36:TYR:CD1	2.55	0.41
9:A:173:LYS:HE3	9:A:173:LYS:HB2	1.76	0.41
9:A:47:VAL:O	9:A:47:VAL:HG23	2.21	0.40
9:A:47:VAL:O	9:A:49:THR:HG23	2.21	0.40
1:B:403[A]:DG:H1'	1:B:404[A]:DT:H5'	2.03	0.40
8:I:508[D]:DA:H2''	8:I:509[D]:DA:C8	2.57	0.40
9:A:132:PHE:O	9:A:133:LYS:O	2.40	0.40
4:E:507[B]:DG:H4'	4:E:508[B]:DG:OP1	2.22	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:A:104:ARG:NE	9:A:104:ARG:NH1[13_555]	1.89	0.31
9:A:186:ARG:NH2	9:A:188:ASP:OD2[5_555]	1.91	0.29
9:A:104:ARG:NH1	9:A:104:ARG:NH1[13_555]	2.09	0.11

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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



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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	A	195/203 (96%)	174 (89%)	16 (8%)	5 (3%)	8	41

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	A	132	PHE
9	A	133	LYS
9	A	124	LEU
9	A	185	ALA
9	A	129	LYS

### 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	
9	A	160/163 (98%)	142 (89%)	18 (11%)	9	32

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

Mol	Chain	Res	Type
9	A	17	VAL
9	A	18	LEU
9	A	55	GLU
9	A	59	LEU
9	A	67	GLN
9	A	127	GLU
9	A	130	ASP
9	A	141	THR
9	A	145	ASP
9	A	149	THR
9	A	156	THR
9	A	158	ASP
9	A	186	ARG
9	A	192	GLU
9	A	194	LEU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
9	A	197	GLU
9	A	199	LEU
9	A	200	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
9	A	13	GLN
9	A	67	GLN
9	A	96	GLN
9	A	100	ASN
9	A	175	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	B	13/13 (100%)	0.86	1 (7%) 13 2	64, 86, 118, 120	13 (100%)
2	C	12/12 (100%)	0.58	0 100 100	69, 86, 102, 112	12 (100%)
3	D	13/13 (100%)	0.88	1 (7%) 13 2	64, 97, 117, 117	13 (100%)
4	E	12/12 (100%)	0.61	0 100 100	64, 97, 105, 110	12 (100%)
5	F	13/13 (100%)	0.84	0 100 100	66, 101, 125, 126	13 (100%)
6	G	12/12 (100%)	0.58	0 100 100	33, 94, 112, 127	12 (100%)
7	H	13/13 (100%)	0.83	0 100 100	69, 91, 122, 126	13 (100%)
8	I	12/12 (100%)	0.57	0 100 100	68, 99, 110, 112	12 (100%)
9	A	199/203 (98%)	-0.20	0 100 100	13, 40, 85, 104	0
All	All	299/303 (98%)	0.11	2 (0%) 84 32	13, 60, 115, 127	100 (33%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	407[A]	DG	2.3
3	D	407[B]	DA	2.3

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.