



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:26 AM UTC

PDB ID : 7OA5 / pdb_00007oa5
Title : RUVA COMPLEXED TO A HOLLIDAY JUNCTION.
Authors : Roe, S.M.; Pearl, L.H.
Deposited on : 2021-04-19
Resolution : 2.38 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

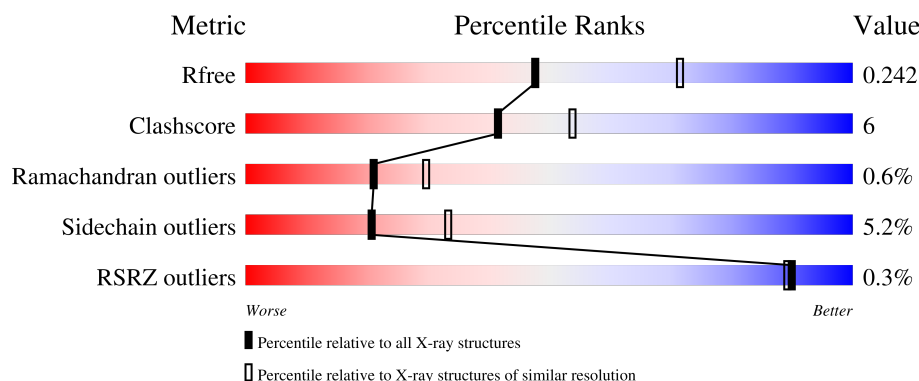
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.38 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}	180053	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

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 of 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	203	
1	B	203	
1	C	203	
1	D	203	
1	E	203	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	203	84% 6% 9%
1	G	203	82% • 13%
1	H	203	83% 8% 9%
2	I	15	100%
3	J	14	7% 93%
4	K	16	6% 94%
5	L	15	20% 80%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11940 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 Holliday junction ATP-dependent DNA helicase RuvA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	181	Total	C	N	O	S	0	1	0
			1267	794	223	246	4			
1	B	186	Total	C	N	O	S	0	0	0
			1321	823	234	260	4			
1	C	184	Total	C	N	O	S	0	1	0
			1281	799	226	252	4			
1	D	184	Total	C	N	O	S	0	0	0
			1301	809	230	258	4			
1	E	182	Total	C	N	O	S	0	0	0
			1259	787	217	251	4			
1	F	184	Total	C	N	O	S	0	1	0
			1303	811	229	259	4			
1	G	177	Total	C	N	O	S	0	1	0
			1238	774	220	240	4			
1	H	184	Total	C	N	O	S	0	1	0
			1292	805	226	257	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	15	Total	C	N	O	P	0	0	0
			305	146	55	90	14			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	J	14	Total	C	N	O	P	0	0	0
			283	135	57	78	13			

- Molecule 4 is a DNA chain called DNA (5'-D(*AP*GP*TP*TP*CP*GP*CP*GP*CP*GP*CP*GP*AP*AP*CP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	K	16	Total	C	N	O	P	0	0	0
			325	155	61	94	15			

- Molecule 5 is a DNA chain called DNA (5'-D(P*GP*TP*TP*CP*GP*CP*GP*CP*GP*CP*GP*AP*AP*CP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	L	15	Total	C	N	O	P	0	0	0
			307	145	56	91	15			

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	K	1	Total	Ca	0	0
			1	1		
6	L	1	Total	Ca	0	0
			1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	58	Total	O	0	0
			58	58		
7	B	43	Total	O	0	0
			43	43		
7	C	63	Total	O	0	0
			63	63		
7	D	48	Total	O	0	0
			48	48		
7	E	73	Total	O	0	0
			73	73		
7	F	46	Total	O	0	0
			46	46		
7	G	64	Total	O	0	0
			64	64		
7	H	52	Total	O	0	0
			52	52		
7	I	3	Total	O	0	0
			3	3		
7	J	1	Total	O	0	0
			1	1		
7	K	3	Total	O	0	0
			3	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	L	2	Total	O	0	0
			2	2		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

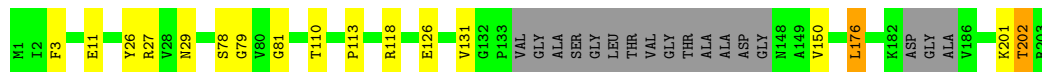
- Molecule 1: Holliday junction ATP-dependent DNA helicase RuvA

Chain A: 



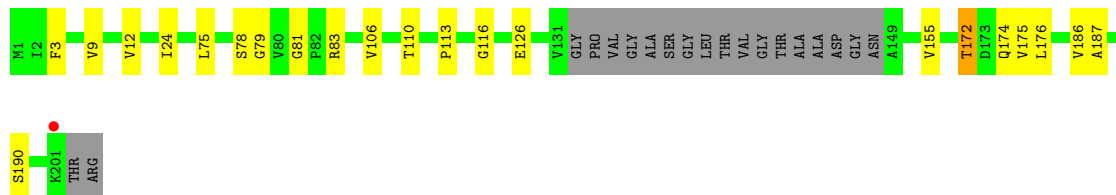
- Molecule 1: Holliday junction ATP-dependent DNA helicase RuvA

Chain B: 



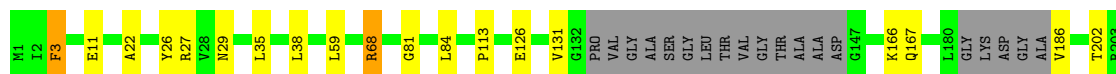
- Molecule 1: Holliday junction ATP-dependent DNA helicase RuvA

Chain C: 



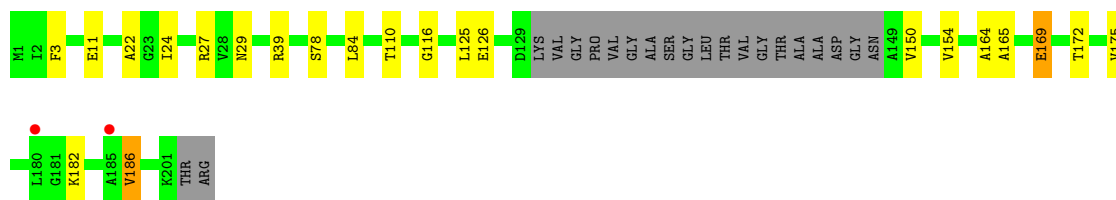
- Molecule 1: Holliday junction ATP-dependent DNA helicase RuvA

Chain D: 



- Molecule 1: Holliday junction ATP-dependent DNA helicase RuvA

Chain E: 



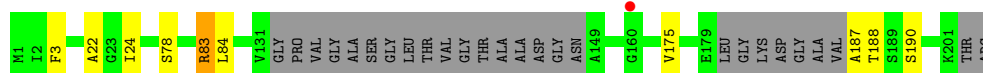
- Molecule 1: Holliday junction ATP-dependent DNA helicase RuvA

Chain F: 84% 6% 9%



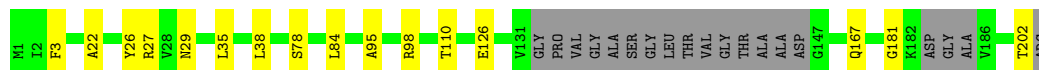
- Molecule 1: Holliday junction ATP-dependent DNA helicase RuvA

Chain G: 82% 13%



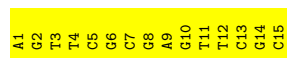
- Molecule 1: Holliday junction ATP-dependent DNA helicase RuvA

Chain H: 83% 8% 9%



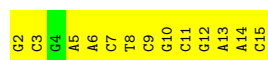
- Molecule 2: DNA (5'-D(*AP*GP*TP*TP*CP*GP*CP*GP*AP*GP*TP*TP*CP*GP*C)-3')

Chain I: 100%



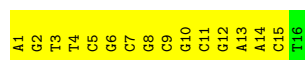
- Molecule 3: DNA (5'-D(*GP*CP*GP*AP*AP*CP*TP*CP*GP*CP*GP*AP*AP*C)-3')

Chain J: 7% 93%



- Molecule 4: DNA (5'-D(*AP*GP*TP*TP*CP*GP*CP*GP*CP*GP*AP*AP*CP*T)-3')

Chain K: 6% 94%



- Molecule 5: DNA (5'-D(P*GP*TP*TP*CP*GP*CP*GP*CP*GP*CP*GP*AP*AP*CP*T)-3')

Chain L:  20% 80%

G2	T3	T4	G5	G6	C7	C8	C9	G10	G11	G12	A13	A14	G15	T16
----	----	----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	141.35Å 141.35Å 106.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	53.06 – 2.38 53.06 – 2.38	Depositor EDS
% Data completeness (in resolution range)	99.4 (53.06-2.38) 99.4 (53.06-2.38)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 2.37Å)	Xtriage
Refinement program	BUSTER 2.10.4	Depositor
R, R_{free}	0.227 , 0.250 0.221 , 0.242	Depositor DCC
R_{free} test set	4597 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	41.3	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 33.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.460 for -h,-k,l 0.467 for h,-h-k,-l 0.466 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11940	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% of the height of the origin peak. No significant pseudotranslation is detected.*

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

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	0.73	1/1279 (0.1%)	1.06	1/1738 (0.1%)
1	B	0.76	0/1330	1.04	2/1804 (0.1%)
1	C	0.72	0/1293	1.02	0/1758
1	D	0.74	0/1309	1.02	0/1776
1	E	0.74	1/1268 (0.1%)	1.06	0/1725
1	F	0.75	0/1314	1.01	0/1783
1	G	0.72	0/1249	1.02	0/1697
1	H	0.76	0/1303	1.02	0/1769
2	I	0.34	0/341	0.59	0/525
3	J	0.46	0/318	0.52	0/489
4	K	0.45	0/364	0.57	0/560
5	L	0.41	0/343	0.54	0/527
All	All	0.71	2/11711 (0.0%)	0.98	3/16151 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	MET	SD-CE	-5.58	1.65	1.79
1	E	186	VAL	CA-C	5.13	1.59	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	201	LYS	CA-C-N	6.96	134.83	121.54
1	B	201	LYS	C-N-CA	6.96	134.83	121.54
1	A	201	LYS	N-CA-C	5.40	117.16	111.28

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	1267	0	1263	16	0
1	B	1321	0	1329	10	0
1	C	1281	0	1264	12	0
1	D	1301	0	1298	9	0
1	E	1259	0	1238	10	0
1	F	1303	0	1292	7	0
1	G	1238	0	1230	6	0
1	H	1292	0	1275	9	0
2	I	305	0	171	44	0
3	J	283	0	154	38	0
4	K	325	0	181	33	0
5	L	307	0	169	35	0
6	K	1	0	0	0	0
6	L	1	0	0	0	0
7	A	58	0	0	0	0
7	B	43	0	0	1	0
7	C	63	0	0	1	0
7	D	48	0	0	0	0
7	E	73	0	0	0	0
7	F	46	0	0	0	0
7	G	64	0	0	0	0
7	H	52	0	0	2	0
7	I	3	0	0	0	0
7	J	1	0	0	0	0
7	K	3	0	0	0	0
7	L	2	0	0	0	0
All	All	11940	0	10864	142	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 6.

All (142) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:9:DC:N4	4:K:8:DG:H1	1.33	1.25

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:3:DT:H3	5:L:14:DA:N6	1.37	1.22
2:I:8:DG:H1	5:L:9:DC:N4	1.43	1.15
4:K:9:DC:N4	5:L:8:DG:H1	1.49	1.09
2:I:9:DA:N6	3:J:8:DT:H3	1.52	1.08
3:J:11:DC:N4	4:K:6:DG:H1	1.52	1.07
2:I:6:DG:H1	5:L:11:DC:N4	1.58	0.99
2:I:13:DC:N4	3:J:3:DC:H42	1.59	0.98
2:I:12:DT:H3	3:J:5:DA:N6	1.61	0.97
2:I:6:DG:H1	5:L:11:DC:H42	0.95	0.94
2:I:9:DA:H61	3:J:8:DT:H3	0.99	0.94
2:I:11:DT:H3	3:J:6:DA:H61	1.11	0.94
2:I:13:DC:H42	3:J:3:DC:H42	1.04	0.93
4:K:11:DC:H42	5:L:6:DG:H1	1.12	0.90
3:J:9:DC:N4	4:K:8:DG:N1	2.17	0.90
2:I:3:DT:H3	5:L:14:DA:H61	1.13	0.88
2:I:11:DT:H3	3:J:6:DA:N6	1.71	0.88
2:I:3:DT:N3	5:L:14:DA:N6	2.20	0.87
2:I:12:DT:N3	3:J:5:DA:N6	2.22	0.87
2:I:13:DC:H42	3:J:3:DC:N4	1.75	0.85
5:L:13:DA:H2''	5:L:14:DA:H5''	1.62	0.82
2:I:13:DC:N4	3:J:3:DC:N4	2.28	0.82
2:I:4:DT:H2''	2:I:5:DC:H5''	1.60	0.81
2:I:3:DT:H3	5:L:14:DA:H62	1.29	0.80
2:I:1:DA:C5'	5:L:16:DT:H3	1.95	0.80
2:I:5:DC:H2''	2:I:6:DG:N7	1.97	0.80
3:J:9:DC:H42	4:K:8:DG:H1	0.82	0.79
1:E:165:ALA:O	1:E:169:GLU:HG2	1.81	0.79
4:K:11:DC:N4	5:L:6:DG:N1	2.29	0.78
4:K:11:DC:N4	5:L:6:DG:H1	1.81	0.77
1:E:116:GLY:HA3	5:L:14:DA:O5'	1.86	0.76
2:I:8:DG:N1	5:L:9:DC:N4	2.26	0.74
3:J:11:DC:H42	4:K:6:DG:H1	0.77	0.73
2:I:12:DT:H3	3:J:5:DA:H61	1.24	0.72
1:E:164:ALA:HB2	2:I:15:DC:O3'	1.89	0.72
3:J:11:DC:H2''	3:J:12:DG:N7	2.05	0.72
1:C:79:GLY:N	3:J:10:DG:OP2	2.17	0.71
2:I:1:DA:H5''	5:L:16:DT:H3	1.54	0.71
1:C:83:ARG:HB2	3:J:11:DC:H5'	1.73	0.69
1:F:84:LEU:HB2	5:L:7:DC:OP1	1.92	0.69
3:J:11:DC:N4	4:K:6:DG:N1	2.23	0.68
1:E:84:LEU:HB2	2:I:7:DC:OP1	1.94	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:84:LEU:HB2	4:K:7:DC:OP1	1.94	0.66
2:I:9:DA:N6	3:J:8:DT:N3	2.29	0.66
1:G:83:ARG:NH1	4:K:6:DG:OP2	2.30	0.64
2:I:6:DG:N1	5:L:11:DC:N4	2.22	0.64
1:F:113:PRO:HA	4:K:15:DC:OP1	1.96	0.64
4:K:13:DA:H2''	4:K:14:DA:H5''	1.79	0.64
1:A:98:ARG:HD3	1:A:133:PRO:HD2	1.80	0.63
1:B:110:THR:O	7:B:301:HOH:O	2.15	0.63
1:H:84:LEU:HB2	3:J:7:DC:OP1	1.98	0.63
1:A:111:ARG:NE	1:B:202:THR:OG1	2.33	0.62
1:E:27:ARG:NH1	1:E:29:ASN:OD1	2.34	0.61
5:L:13:DA:C2'	5:L:14:DA:H5''	2.31	0.61
2:I:6:DG:N2	5:L:11:DC:N3	2.44	0.60
1:A:27:ARG:NH1	1:A:29:ASN:OD1	2.34	0.60
2:I:8:DG:H1	5:L:9:DC:H42	0.71	0.59
1:F:27:ARG:NH1	1:F:29:ASN:OD1	2.35	0.59
3:J:13:DA:H1'	3:J:14:DA:H5'	1.84	0.59
1:D:84:LEU:HB2	4:K:11:DC:OP2	2.02	0.59
2:I:4:DT:H2''	2:I:5:DC:C5'	2.30	0.59
1:B:27:ARG:NH1	1:B:29:ASN:OD1	2.36	0.58
1:H:84:LEU:N	3:J:7:DC:OP1	2.30	0.58
3:J:11:DC:H2''	3:J:12:DG:C8	2.39	0.58
1:H:27:ARG:NH1	1:H:29:ASN:OD1	2.35	0.58
1:D:27:ARG:NH1	1:D:29:ASN:OD1	2.36	0.57
2:I:5:DC:H2''	2:I:6:DG:C8	2.40	0.56
1:H:95:ALA:HA	1:H:98:ARG:HB3	1.88	0.55
4:K:2:DG:H2''	4:K:3:DT:H71	1.87	0.55
1:A:24:ILE:HD11	1:B:26:TYR:CE2	2.41	0.55
1:A:116:GLY:N	2:I:4:DT:OP2	2.40	0.54
1:A:166:LYS:O	1:A:170:GLU:HG2	2.08	0.54
1:G:24:ILE:HD11	1:H:26:TYR:CE2	2.43	0.54
1:H:110:THR:O	7:H:301:HOH:O	2.19	0.53
2:I:2:DG:H2''	2:I:3:DT:C5	2.44	0.53
1:B:81:GLY:HA3	2:I:10:DG:C3'	2.39	0.53
4:K:3:DT:O5'	4:K:3:DT:H6	1.92	0.51
1:C:116:GLY:N	4:K:4:DT:OP2	2.42	0.51
7:H:301:HOH:O	2:I:15:DC:OP1	2.19	0.51
3:J:15:DC:H2''	4:K:1:DA:H62	1.76	0.51
4:K:12:DG:H2''	4:K:13:DA:C8	2.46	0.51
5:L:11:DC:H2''	5:L:12:DG:C8	2.46	0.50
1:E:24:ILE:HD11	1:F:26:TYR:CE2	2.47	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:154:VAL:HG12	1:E:172:THR:HG22	1.93	0.50
1:E:154:VAL:CG1	1:E:172:THR:HG22	2.43	0.49
1:D:81:GLY:HA3	4:K:10:DG:H4'	1.94	0.49
1:C:186:VAL:O	1:C:190:SER:HB3	2.13	0.49
1:C:24:ILE:HD11	1:D:26:TYR:CE2	2.47	0.49
1:F:22:ALA:HB1	1:G:22:ALA:HB2	1.94	0.49
1:A:83:ARG:HB2	5:L:11:DC:OP1	2.13	0.48
1:A:128:ARG:O	1:A:129:ASP:HB2	2.13	0.48
1:D:113:PRO:HA	5:L:3:DT:OP2	2.13	0.48
3:J:15:DC:H2''	4:K:1:DA:N6	2.27	0.48
4:K:11:DC:N4	5:L:6:DG:C6	2.81	0.48
3:J:11:DC:C2'	3:J:12:DG:N7	2.76	0.47
1:B:150:VAL:HG12	1:B:176:LEU:HD21	1.96	0.47
3:J:10:DG:O6	4:K:7:DC:N3	2.47	0.47
1:B:79:GLY:N	2:I:10:DG:OP2	2.44	0.47
2:I:14:DG:O6	3:J:3:DC:N3	2.48	0.47
1:G:187:ALA:HB3	1:G:190:SER:HB2	1.98	0.46
4:K:3:DT:H2'	4:K:4:DT:C6	2.50	0.46
4:K:13:DA:N1	5:L:4:DT:O4	2.48	0.46
1:F:3:PHE:CD2	1:F:68:ARG:NH1	2.84	0.46
1:H:95:ALA:HA	1:H:98:ARG:CB	2.46	0.45
1:A:81:GLY:HA3	5:L:10:DG:O3'	2.16	0.45
2:I:2:DG:H2''	2:I:3:DT:C6	2.52	0.45
4:K:12:DG:H2''	4:K:13:DA:N7	2.32	0.45
1:C:110:THR:O	7:C:301:HOH:O	2.21	0.45
4:K:5:DC:H2''	4:K:6:DG:O5'	2.17	0.45
4:K:9:DC:N4	5:L:8:DG:N1	2.27	0.45
1:C:79:GLY:C	3:J:10:DG:H5'	2.41	0.45
1:C:155:VAL:HG23	1:C:172:THR:HG21	1.99	0.45
2:I:15:DC:N3	3:J:2:DG:O6	2.49	0.45
1:A:81:GLY:CA	5:L:10:DG:H4'	2.48	0.44
1:D:3:PHE:CD2	1:D:68:ARG:NH2	2.85	0.44
4:K:9:DC:H42	5:L:8:DG:H1	0.63	0.44
1:F:35:LEU:HD23	1:F:38:LEU:HD12	1.99	0.44
1:A:22:ALA:HB2	1:D:22:ALA:HB1	2.00	0.43
1:A:81:GLY:HA3	5:L:10:DG:H4'	1.99	0.43
1:A:83:ARG:HB2	5:L:11:DC:H5'	1.99	0.43
1:C:106:VAL:O	1:C:110:THR:HG23	2.17	0.43
1:D:35:LEU:HD23	1:D:38:LEU:HD12	2.00	0.43
1:H:35:LEU:HD23	1:H:38:LEU:HD12	2.00	0.43
1:G:175:VAL:O	1:G:175:VAL:HG12	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:PRO:HA	3:J:3:DC:OP2	2.18	0.43
1:C:81:GLY:HA3	3:J:10:DG:O3'	2.18	0.43
1:B:81:GLY:HA3	2:I:10:DG:O3'	2.19	0.43
5:L:13:DA:C3'	5:L:14:DA:H5''	2.49	0.42
2:I:10:DG:O6	3:J:7:DC:N3	2.52	0.42
1:A:128:ARG:O	1:A:129:ASP:CB	2.68	0.42
2:I:11:DT:N3	3:J:6:DA:N6	2.46	0.42
1:E:22:ALA:HB2	1:H:22:ALA:HB1	2.01	0.41
1:A:1:MET:HE2	1:D:59:LEU:HG	2.02	0.41
1:C:9:VAL:HG11	1:C:12:VAL:HG22	2.03	0.41
3:J:11:DC:N4	4:K:5:DC:N4	2.69	0.41
1:B:118:ARG:NH1	1:E:125:LEU:O	2.47	0.41
1:C:113:PRO:HA	4:K:3:DT:OP2	2.21	0.40
3:J:12:DG:H2''	3:J:13:DA:C8	2.57	0.40
4:K:1:DA:H2'	4:K:2:DG:C4	2.56	0.40
2:I:6:DG:C6	5:L:11:DC:N4	2.85	0.40
1:A:106:VAL:HG13	1:A:120:ALA:HB3	2.03	0.40
2:I:1:DA:H5''	5:L:16:DT:N3	2.30	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	176/203 (87%)	171 (97%)	2 (1%)	3 (2%)	7	9
1	B	180/203 (89%)	174 (97%)	5 (3%)	1 (1%)	21	30
1	C	181/203 (89%)	174 (96%)	5 (3%)	2 (1%)	11	16
1	D	178/203 (88%)	176 (99%)	2 (1%)	0	100	100
1	E	178/203 (88%)	170 (96%)	6 (3%)	2 (1%)	11	16
1	F	179/203 (88%)	177 (99%)	2 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	172/203 (85%)	168 (98%)	4 (2%)	0	100	100
1	H	179/203 (88%)	175 (98%)	3 (2%)	1 (1%)	21	30
All	All	1423/1624 (88%)	1385 (97%)	29 (2%)	9 (1%)	21	30

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	129	ASP
1	B	202	THR
1	A	187	ALA
1	E	182	LYS
1	E	186	VAL
1	C	187	ALA
1	A	132	GLY
1	C	175	VAL
1	H	181	GLY

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	120/146 (82%)	114 (95%)	6 (5%)	22	35
1	B	130/146 (89%)	124 (95%)	6 (5%)	24	38
1	C	120/146 (82%)	113 (94%)	7 (6%)	18	29
1	D	127/146 (87%)	118 (93%)	9 (7%)	13	21
1	E	118/146 (81%)	109 (92%)	9 (8%)	12	19
1	F	126/146 (86%)	121 (96%)	5 (4%)	28	44
1	G	117/146 (80%)	113 (97%)	4 (3%)	32	51
1	H	123/146 (84%)	118 (96%)	5 (4%)	27	43
All	All	981/1168 (84%)	930 (95%)	51 (5%)	21	33

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	PHE
1	A	78	SER
1	A	126	GLU
1	A	131	VAL
1	A	150	VAL
1	A	175	VAL
1	B	3	PHE
1	B	11	GLU
1	B	78	SER
1	B	126	GLU
1	B	131	VAL
1	B	176	LEU
1	C	3	PHE
1	C	75	LEU
1	C	78	SER
1	C	126	GLU
1	C	172	THR
1	C	174	GLN
1	C	176	LEU
1	D	3	PHE
1	D	11	GLU
1	D	68	ARG
1	D	126	GLU
1	D	131	VAL
1	D	166	LYS
1	D	167	GLN
1	D	186	VAL
1	D	202	THR
1	E	3	PHE
1	E	11	GLU
1	E	39	ARG
1	E	78	SER
1	E	110	THR
1	E	126	GLU
1	E	150	VAL
1	E	169	GLU
1	E	175	VAL
1	F	3	PHE
1	F	11	GLU
1	F	78	SER
1	F	126	GLU
1	F	179	GLU
1	G	3	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	78	SER
1	G	83	ARG
1	G	188	THR
1	H	3	PHE
1	H	78	SER
1	H	126	GLU
1	H	167	GLN
1	H	202	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	174	GLN
1	D	92	HIS
1	E	40	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 [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	181/203 (89%)	-0.71	1 (0%) 85 85	20, 42, 97, 106	1 (0%)
1	B	186/203 (91%)	-0.82	0 100 100	25, 46, 75, 97	0
1	C	184/203 (90%)	-0.61	1 (0%) 87 86	20, 42, 114, 120	1 (0%)
1	D	184/203 (90%)	-0.79	0 100 100	26, 45, 74, 86	0
1	E	182/203 (89%)	-0.64	2 (1%) 78 77	25, 42, 108, 118	0
1	F	184/203 (90%)	-0.80	0 100 100	22, 45, 74, 93	1 (0%)
1	G	177/203 (87%)	-0.74	1 (0%) 85 85	20, 41, 98, 118	1 (0%)
1	H	184/203 (90%)	-0.82	0 100 100	22, 45, 72, 87	1 (0%)
2	I	15/15 (100%)	-0.48	0 100 100	83, 96, 128, 129	0
3	J	14/14 (100%)	-0.56	0 100 100	78, 97, 121, 122	0
4	K	16/16 (100%)	-0.59	0 100 100	85, 99, 140, 143	0
5	L	15/15 (100%)	-0.56	0 100 100	92, 102, 131, 134	0
All	All	1522/1684 (90%)	-0.73	5 (0%) 90 89	20, 45, 102, 143	5 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	180	LEU	2.8
1	C	201	LYS	2.7
1	E	185	ALA	2.3
1	A	163	PHE	2.1
1	G	160	GLY	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	CA	K	101	1/1	0.99	0.06	72,72,72,72	0
6	CA	L	101	1/1	0.99	0.06	75,75,75,75	0

6.5 Other polymers [i](#)

There are no such residues in this entry.