



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 06:34 am BST

PDB ID : 3ULP
Title : Plasmodium falciparum SSB complex with ssDNA
Authors : Antony, E.; Lohman, T.M.; Korolev, S.
Deposited on : 2011-11-11
Resolution : 2.10 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

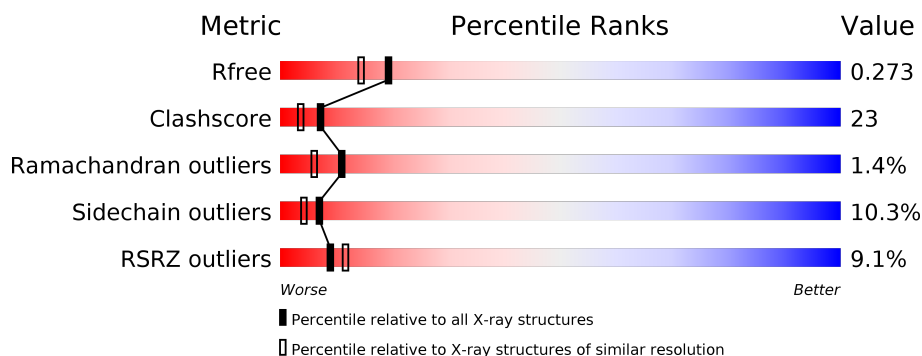
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	124	<div> <div>5%</div> <div>63%</div> <div>26%</div> <div>8%</div> </div>
1	B	124	<div> <div>11%</div> <div>59%</div> <div>26%</div> <div>6%</div> <div>8%</div> </div>
1	C	124	<div> <div>6%</div> <div>59%</div> <div>30%</div> <div>5%</div> <div>6%</div> </div>
1	D	124	<div> <div>10%</div> <div>59%</div> <div>24%</div> <div>7%</div> <div>9%</div> </div>
2	Q	35	<div> <div>9%</div> <div>26%</div> <div>26%</div> <div>20%</div> <div>29%</div> </div>
2	R	35	<div> <div>9%</div> <div>17%</div> <div>46%</div> <div>9%</div> <div>29%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4886 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 Single-strand binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	114	Total	C	N	O	S	0	0	0
			918	580	168	168	2			
1	B	114	Total	C	N	O	S	0	0	0
			898	568	161	167	2			
1	C	116	Total	C	N	O	S	0	0	0
			936	592	171	171	2			
1	D	113	Total	C	N	O	S	0	0	0
			886	566	159	159	2			

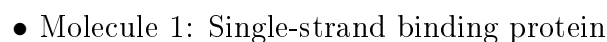
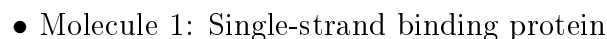
- Molecule 2 is a DNA chain called DNA (35-MER).

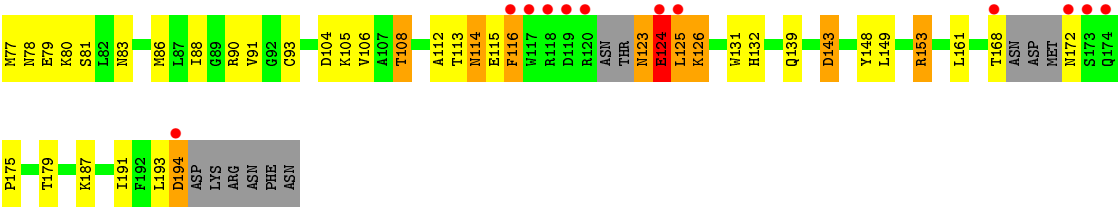
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	R	25	Total	C	N	O	P	0	1	0
			520	260	52	182	26			
2	Q	25	Total	C	N	O	P	0	0	0
			500	250	50	175	25			

- Molecule 3 is water.

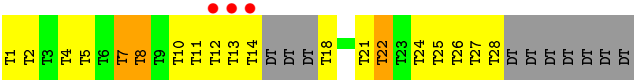
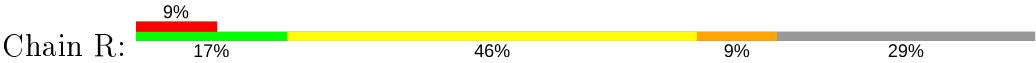
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	47	Total	O	0	0
			47	47		
3	B	35	Total	O	0	0
			35	35		
3	C	49	Total	O	0	0
			49	49		
3	D	44	Total	O	0	0
			44	44		
3	R	24	Total	O	0	0
			24	24		
3	Q	29	Total	O	0	0
			29	29		

- Molecule 1: Single-strand binding protein

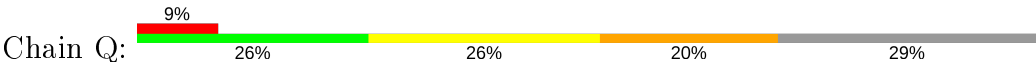




● Molecule 2: DNA (35-MER)



● Molecule 2: DNA (35-MER)



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	118.02Å 82.79Å 87.56Å 90.00° 99.57° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10 26.85 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.2 (30.00-2.10) 99.1 (26.85-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.88 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.218 , 0.276 0.216 , 0.273	Depositor DCC
R_{free} test set	2442 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	33.1	Xtriage
Anisotropy	0.400	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4886	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.17% 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

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	0.49	0/932	0.71	2/1255 (0.2%)
1	B	0.45	0/911	0.66	0/1228
1	C	0.49	0/951	0.70	1/1281 (0.1%)
1	D	0.50	0/900	0.67	0/1211
2	Q	0.82	0/548	1.83	14/842 (1.7%)
2	R	0.80	0/570	1.75	9/876 (1.0%)
All	All	0.58	0/4812	1.08	26/6693 (0.4%)

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
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	2
All	All	0	5

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	8	DT	N3-C4-O4	8.46	124.98	119.90
2	R	8	DT	C5-C4-O4	-8.43	119.00	124.90
2	Q	8	DT	O4'-C1'-N1	-8.28	102.20	108.00
2	Q	1	DT	O4'-C4'-C3'	-8.26	101.04	106.00
2	R	1	DT	O4'-C4'-C3'	-8.02	101.19	106.00
2	Q	8	DT	C5-C4-O4	-7.54	119.62	124.90
2	R	8	DT	O4'-C1'-N1	-7.50	102.75	108.00
2	Q	24	DT	P-O3'-C3'	7.34	128.51	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	26	DT	O4'-C4'-C3'	-6.95	101.72	104.50
2	Q	8	DT	N3-C4-O4	6.72	123.93	119.90
1	C	90	ARG	NE-CZ-NH1	6.43	123.52	120.30
2	Q	23	DT	C5-C4-O4	-6.43	120.40	124.90
2	R	7	DT	O4'-C1'-N1	6.33	112.43	108.00
2	Q	19	DT	C5-C4-O4	-6.29	120.50	124.90
1	A	189	ASP	CB-CG-OD1	5.51	123.26	118.30
2	Q	18	DT	C5-C4-O4	-5.50	121.05	124.90
2	R	21	DT	C5-C4-O4	-5.49	121.06	124.90
2	Q	9	DT	O5'-P-OP1	-5.49	100.76	105.70
1	A	164	ARG	NE-CZ-NH2	-5.32	117.64	120.30
2	R	22	DT	C6-C5-C7	-5.31	119.71	122.90
2	Q	2	DT	O4'-C1'-N1	5.31	111.72	108.00
2	R	26	DT	C5-C4-O4	-5.26	121.22	124.90
2	R	7	DT	C1'-O4'-C4'	-5.13	104.97	110.10
2	Q	8	DT	C2-N3-C4	-5.09	124.14	127.20
2	Q	25	DT	O4'-C1'-N1	-5.06	104.46	108.00
2	Q	26	DT	O4'-C1'-N1	5.06	111.54	108.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	167	HIS	Peptide
1	B	124	GLU	Peptide
1	C	121	ASN	Peptide
1	D	123	ASN	Peptide
1	D	124	GLU	Peptide

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	918	0	926	30	1
1	B	898	0	881	44	0
1	C	936	0	936	66	1
1	D	886	0	875	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Q	500	0	302	24	1
2	R	520	0	314	28	1
3	A	47	0	0	3	0
3	B	35	0	0	2	0
3	C	49	0	0	13	0
3	D	44	0	0	5	0
3	Q	29	0	0	8	0
3	R	24	0	0	8	0
All	All	4886	0	4234	201	2

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 23.

All (201) 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:A:77:MET:N	2:R:27:DT:H3	1.21	1.34
1:D:77:MET:O	2:Q:11:DT:C7	1.75	1.33
2:R:18[A]:DT:H73	3:R:239:HOH:O	1.33	1.27
1:B:163:THR:HG22	1:B:179:THR:HG22	1.21	1.17
1:A:153:ARG:HH11	1:A:153:ARG:CG	1.58	1.16
1:C:168:THR:N	1:C:169:ASN:HA	1.45	1.14
1:C:168:THR:H	1:C:169:ASN:CA	1.60	1.14
1:B:153:ARG:CG	1:B:153:ARG:HH11	1.61	1.12
1:A:153:ARG:NH1	1:A:153:ARG:HG2	1.42	1.12
2:R:7:DT:H2''	2:R:8:DT:OP2	1.47	1.08
1:D:77:MET:O	2:Q:11:DT:H71	0.90	1.05
2:R:18[B]:DT:H2'	3:R:161:HOH:O	1.59	1.01
1:A:77:MET:N	2:R:27:DT:N3	2.06	1.01
1:C:122:THR:CG2	1:C:124:GLU:HB3	1.92	1.00
1:C:122:THR:HG22	1:C:124:GLU:H	1.27	0.98
1:C:122:THR:CG2	1:C:124:GLU:H	1.77	0.97
1:C:173:SER:HB3	3:C:231:HOH:O	1.65	0.96
1:B:179:THR:HG23	3:B:221:HOH:O	1.66	0.95
2:Q:18:DT:H2'	3:Q:196:HOH:O	1.64	0.95
1:C:122:THR:HG21	1:C:124:GLU:HB3	1.49	0.94
1:A:78:ASN:HB2	2:R:28:DT:O2	1.69	0.93
1:B:153:ARG:HG3	1:B:153:ARG:HH11	1.33	0.92
1:B:163:THR:CG2	1:B:179:THR:HG22	1.98	0.92
1:B:153:ARG:HG2	1:B:153:ARG:HH11	1.34	0.92
1:C:105:LYS:H	1:C:139:GLN:HE22	1.11	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:ASN:HB3	3:C:217:HOH:O	1.69	0.90
1:A:78:ASN:HD22	2:R:28:DT:H3	1.19	0.90
1:C:78:ASN:ND2	2:Q:27:DT:H3	1.69	0.89
1:C:78:ASN:HD22	2:Q:27:DT:H3	1.17	0.88
2:R:24:DT:H2"	2:R:25:DT:OP2	1.71	0.88
1:A:164:ARG:NH2	2:R:5:DT:O2	2.06	0.88
1:C:113:THR:CG2	1:C:132:HIS:HE1	1.89	0.85
1:D:77:MET:C	2:Q:11:DT:H71	1.95	0.85
1:C:113:THR:HG22	1:C:132:HIS:HE1	1.40	0.84
1:C:167:HIS:HA	1:C:168:THR:CB	2.07	0.84
1:B:164:ARG:NH2	2:R:22:DT:O2	2.10	0.84
1:A:105:LYS:H	1:A:139:GLN:HE22	1.22	0.82
1:C:153:ARG:HH11	1:C:153:ARG:CG	1.93	0.82
1:D:168:THR:HG22	1:D:172:ASN:N	1.94	0.81
1:D:193:LEU:O	1:D:194:ASP:CB	2.28	0.81
1:D:153:ARG:CG	1:D:153:ARG:HH11	1.95	0.79
1:C:113:THR:HG23	3:D:214:HOH:O	1.82	0.79
1:C:193:LEU:C	1:C:194:ASP:OD1	2.21	0.79
1:B:105:LYS:H	1:B:139:GLN:HE22	1.30	0.79
1:D:78:ASN:HA	2:Q:11:DT:H72	1.64	0.78
1:B:153:ARG:HG2	1:B:153:ARG:NH1	1.94	0.78
1:D:78:ASN:HA	2:Q:11:DT:C7	2.14	0.78
3:C:227:HOH:O	1:D:116:PHE:CE2	2.37	0.77
1:C:167:HIS:CA	1:C:168:THR:CB	2.63	0.77
1:D:153:ARG:HE	2:R:12:DT:H73	1.47	0.77
2:R:18[A]:DT:C7	3:R:239:HOH:O	2.07	0.77
1:B:164:ARG:NH1	1:B:178:ILE:HD11	1.99	0.77
2:Q:29:DT:H5"	2:Q:29:DT:C6	2.20	0.75
1:D:105:LYS:H	1:D:139:GLN:HE22	1.35	0.75
1:B:163:THR:HG22	1:B:179:THR:CG2	2.10	0.74
1:C:153:ARG:HG2	1:C:153:ARG:HH11	1.52	0.73
1:C:173:SER:HB2	3:C:220:HOH:O	1.88	0.73
1:C:79:GLU:OE1	1:D:90:ARG:HD3	1.87	0.73
1:C:113:THR:HG22	1:C:132:HIS:CE1	2.23	0.72
3:C:227:HOH:O	1:D:116:PHE:CD2	2.42	0.72
1:D:153:ARG:HG2	1:D:153:ARG:HH11	1.52	0.72
1:B:153:ARG:CG	1:B:153:ARG:NH1	2.33	0.72
1:C:78:ASN:HB2	3:C:227:HOH:O	1.90	0.72
1:B:165:LYS:NZ	1:B:177:GLN:NE2	2.38	0.71
1:B:80:LYS:HD2	1:D:191:ILE:HG12	1.70	0.71
1:A:164:ARG:HG2	3:A:215:HOH:O	1.89	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:168:THR:N	1:C:169:ASN:CA	2.32	0.70
1:C:153:ARG:HG2	1:C:153:ARG:NH1	2.04	0.70
2:R:18[A]:DT:H6	3:R:162:HOH:O	1.74	0.70
1:C:180:GLU:HB2	3:C:223:HOH:O	1.93	0.69
1:D:193:LEU:O	1:D:194:ASP:HB3	1.91	0.69
1:C:193:LEU:O	1:C:194:ASP:OD1	2.10	0.69
1:C:122:THR:CG2	1:C:124:GLU:CB	2.68	0.68
1:C:168:THR:H	1:C:169:ASN:HA	0.67	0.68
1:C:162:HIS:HB2	3:C:223:HOH:O	1.94	0.67
1:B:165:LYS:HZ2	1:B:177:GLN:NE2	1.93	0.67
1:B:165:LYS:NZ	1:B:177:GLN:HE21	1.93	0.66
1:C:122:THR:HG22	1:C:124:GLU:N	2.07	0.65
1:A:113:THR:OG1	1:A:132:HIS:HE1	1.79	0.64
2:R:18[B]:DT:P	3:R:162:HOH:O	2.55	0.64
1:C:153:ARG:HH11	1:C:153:ARG:CB	2.11	0.63
1:D:153:ARG:NH1	1:D:153:ARG:HG2	2.13	0.63
1:D:153:ARG:HH11	1:D:153:ARG:CB	2.11	0.62
1:D:153:ARG:HE	2:R:12:DT:C7	2.12	0.62
1:C:90:ARG:HD3	1:D:79:GLU:OE1	1.98	0.62
1:C:120:ARG:HD3	1:D:104:ASP:OD2	1.99	0.61
1:C:194:ASP:OD1	1:C:194:ASP:N	2.32	0.61
2:R:12:DT:H4'	2:R:13:DT:OP2	1.99	0.61
1:D:124:GLU:HA	1:D:125:LEU:CB	2.31	0.61
2:Q:7:DT:C5'	3:Q:190:HOH:O	2.47	0.61
1:C:105:LYS:H	1:C:139:GLN:NE2	1.92	0.60
1:B:108:THR:HG23	3:R:151:HOH:O	2.01	0.60
1:A:153:ARG:HH11	1:A:153:ARG:HG2	0.64	0.60
1:B:108:THR:CG2	3:R:151:HOH:O	2.49	0.60
1:C:122:THR:HG23	1:C:124:GLU:H	1.63	0.59
2:Q:29:DT:C6	2:Q:29:DT:C5'	2.85	0.59
1:B:154:ARG:HB3	1:B:194:ASP:HB2	1.85	0.59
1:D:90:ARG:CZ	2:Q:27:DT:H4'	2.33	0.59
1:D:193:LEU:O	1:D:194:ASP:CG	2.41	0.58
1:D:106:VAL:HG11	2:Q:19:DT:H72	1.85	0.58
3:D:216:HOH:O	2:Q:18:DT:H73	2.04	0.58
1:A:153:ARG:NH1	1:A:153:ARG:CG	2.31	0.58
1:C:119:ASP:HB3	1:C:122:THR:HG22	1.86	0.58
1:B:90:ARG:CZ	2:R:27:DT:H4'	2.34	0.58
1:C:126:LYS:HE2	3:C:207:HOH:O	2.03	0.57
1:B:153:ARG:HG3	1:B:153:ARG:NH1	2.11	0.57
2:Q:7:DT:H5''	3:Q:190:HOH:O	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:THR:C	1:B:124:GLU:H	2.09	0.56
1:C:122:THR:CG2	1:C:124:GLU:N	2.59	0.56
1:C:153:ARG:HH11	1:C:153:ARG:HB3	1.71	0.56
2:R:24:DT:C2'	2:R:25:DT:OP2	2.50	0.56
1:C:167:HIS:CB	1:C:168:THR:CB	2.83	0.55
2:Q:1:DT:H2'	2:Q:2:DT:OP2	2.07	0.55
1:A:79:GLU:OE1	1:B:90:ARG:HD3	2.07	0.55
1:D:148:TYR:O	2:R:12:DT:H73	2.08	0.54
1:C:79:GLU:O	1:D:114:ASN:OD1	2.26	0.53
1:D:153:ARG:HH11	1:D:153:ARG:HB3	1.73	0.53
1:C:88:ILE:O	1:D:81:SER:HB2	2.08	0.53
1:D:161:LEU:HD11	1:D:179:THR:CG2	2.39	0.53
1:D:123:ASN:O	1:D:124:GLU:O	2.27	0.53
1:B:191:ILE:HG12	1:D:80:LYS:HD2	1.90	0.53
1:B:193:LEU:O	1:B:194:ASP:CB	2.54	0.53
2:R:7:DT:C2'	2:R:8:DT:OP2	2.36	0.53
1:C:147:LYS:O	1:C:150:ARG:NH2	2.41	0.52
1:B:105:LYS:H	1:B:139:GLN:NE2	2.02	0.52
1:D:132:HIS:HD2	3:D:35:HOH:O	1.93	0.51
1:C:113:THR:HG21	1:C:132:HIS:HE1	1.71	0.51
1:A:78:ASN:ND2	2:R:28:DT:H3	1.99	0.50
1:A:105:LYS:H	1:A:139:GLN:NE2	2.00	0.50
1:A:128:LYS:HD3	2:R:18[B]:DT:O4	2.12	0.50
1:C:98:LYS:HD3	2:Q:2:DT:O4	2.12	0.50
1:A:160:SER:HB3	1:A:162:HIS:NE2	2.27	0.50
1:B:165:LYS:HZ3	1:B:177:GLN:HE21	1.59	0.50
1:C:122:THR:HG23	1:C:124:GLU:CB	2.41	0.50
1:C:167:HIS:HB2	1:C:168:THR:CB	2.42	0.49
1:A:122:THR:OG1	1:A:124:GLU:HG2	2.13	0.49
1:C:84:LYS:HD2	1:C:86:MET:CE	2.43	0.49
1:C:162:HIS:CE1	1:D:115:GLU:HG3	2.47	0.49
1:A:112:ALA:HB2	1:A:131:TRP:CZ3	2.48	0.49
1:D:143:ASP:CG	3:D:207:HOH:O	2.49	0.49
1:D:80:LYS:HG3	2:Q:13:DT:H4'	1.94	0.49
2:Q:7:DT:H5'	3:Q:190:HOH:O	2.11	0.49
1:C:90:ARG:CZ	2:Q:10:DT:H4'	2.43	0.48
1:B:138:ASP:O	1:B:142:VAL:HG23	2.12	0.48
1:A:119:ASP:HB2	1:A:126:LYS:HD2	1.96	0.48
2:R:10:DT:H2'	2:R:11:DT:C6	2.48	0.48
1:A:185:TYR:CB	3:A:218:HOH:O	2.61	0.47
1:C:93:CYS:SG	3:Q:69:HOH:O	2.20	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:SER:HB2	1:D:88:ILE:O	2.15	0.47
1:C:84:LYS:HD2	1:C:86:MET:HE1	1.97	0.47
1:D:132:HIS:CD2	3:D:35:HOH:O	2.67	0.47
1:A:96:ASP:OD2	1:A:98:LYS:HE3	2.15	0.46
1:C:126:LYS:CE	3:C:207:HOH:O	2.62	0.46
2:R:2:DT:H73	2:R:4:DT:O2	2.15	0.46
1:B:122:THR:CG2	1:B:124:GLU:HG2	2.46	0.46
2:Q:1:DT:C2'	2:Q:2:DT:OP2	2.63	0.46
1:C:150:ARG:NH1	3:C:64:HOH:O	2.48	0.45
1:A:112:ALA:HB2	1:A:131:TRP:CH2	2.51	0.45
1:C:119:ASP:HB2	1:C:126:LYS:HD2	1.97	0.45
3:C:222:HOH:O	1:D:187:LYS:HD3	2.17	0.44
1:D:91:VAL:HG21	1:D:149:LEU:HD11	2.00	0.44
1:D:108:THR:HG23	3:Q:127:HOH:O	2.18	0.44
1:A:87:LEU:HD23	1:B:83:ASN:HA	1.99	0.44
1:B:137:TYR:CE1	2:R:18[B]:DT:H1'	2.53	0.44
2:R:14:DT:O2	2:R:14:DT:C2'	2.65	0.44
1:B:122:THR:O	1:B:124:GLU:N	2.48	0.44
2:Q:24:DT:H2''	2:Q:25:DT:OP2	2.18	0.43
1:A:132:HIS:HB3	1:A:181:ILE:HD13	2.00	0.43
1:B:164:ARG:HD3	1:B:180:GLU:OE1	2.19	0.43
1:B:140:ASN:CG	3:B:207:HOH:O	2.57	0.43
1:B:169:ASN:O	1:B:170:ASP:C	2.57	0.43
1:B:181:ILE:N	1:B:181:ILE:HD12	2.34	0.43
1:C:85:ILE:CD1	1:D:161:LEU:HD22	2.48	0.43
1:B:166:TRP:N	1:B:166:TRP:CD1	2.86	0.43
1:A:124:GLU:HG2	3:A:76:HOH:O	2.17	0.43
1:C:176:LYS:HE3	3:C:225:HOH:O	2.19	0.43
1:D:124:GLU:CB	1:D:126:LYS:HB2	2.49	0.43
1:D:93:CYS:SG	3:Q:245:HOH:O	2.21	0.42
1:D:113:THR:OG1	1:D:132:HIS:HE1	2.02	0.42
1:A:118:ARG:HD3	1:A:123:ASN:O	2.19	0.42
1:B:113:THR:OG1	1:B:132:HIS:HE1	2.02	0.42
1:B:168:THR:O	1:B:169:ASN:C	2.58	0.42
1:A:86:MET:SD	1:D:86:MET:CE	3.08	0.42
1:C:119:ASP:HB3	1:C:122:THR:CG2	2.50	0.41
1:A:178:ILE:HD12	2:R:5:DT:H2''	2.02	0.41
1:A:138:ASP:O	1:A:142:VAL:HG23	2.20	0.41
1:C:138:ASP:O	1:C:142:VAL:HG23	2.20	0.41
1:D:194:ASP:C	1:D:194:ASP:OD2	2.58	0.41
1:B:165:LYS:HZ3	1:B:177:GLN:NE2	2.17	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:LEU:HD23	1:D:83:ASN:HA	2.02	0.41
1:B:122:THR:HG22	1:B:124:GLU:HG2	2.03	0.41
1:C:92:GLY:HA3	1:C:131:TRP:CZ3	2.55	0.41
1:C:108:THR:HG22	3:Q:57:HOH:O	2.21	0.41
1:D:112:ALA:HB2	1:D:131:TRP:CH2	2.57	0.41
1:B:193:LEU:O	1:B:194:ASP:CG	2.59	0.40
1:D:112:ALA:HB2	1:D:131:TRP:CZ3	2.56	0.40
1:B:80:LYS:CD	1:D:191:ILE:HG12	2.47	0.40
1:C:162:HIS:HE1	1:D:115:GLU:HG3	1.83	0.40
1:B:144:LEU:HD13	2:Q:13:DT:H3'	2.02	0.40
2:R:18[B]:DT:C2'	3:R:161:HOH:O	2.38	0.40
2:Q:10:DT:H2'	2:Q:11:DT:C2	2.56	0.40

All (2) 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	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:THR:O	2:Q:8:DT:C7[4_545]	1.78	0.42
1:C:122:THR:O	2:R:8:DT:C7[4_555]	1.91	0.29

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	
1	A	110/124 (89%)	107 (97%)	3 (3%)	0	100	100
1	B	108/124 (87%)	103 (95%)	4 (4%)	1 (1%)	17	12
1	C	112/124 (90%)	108 (96%)	2 (2%)	2 (2%)	8	4
1	D	107/124 (86%)	100 (94%)	4 (4%)	3 (3%)	5	1
All	All	437/496 (88%)	418 (96%)	13 (3%)	6 (1%)	11	6

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	168	THR
1	D	125	LEU
1	D	124	GLU
1	B	123	ASN
1	C	174	GLN
1	D	175	PRO

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	100/115 (87%)	91 (91%)	9 (9%)	9	6
1	B	95/115 (83%)	78 (82%)	17 (18%)	2	1
1	C	101/115 (88%)	94 (93%)	7 (7%)	15	12
1	D	92/115 (80%)	85 (92%)	7 (8%)	13	10
All	All	388/460 (84%)	348 (90%)	40 (10%)	7	4

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	LYS
1	A	143	ASP
1	A	147	LYS
1	A	153	ARG
1	A	164	ARG
1	A	167	HIS
1	A	173	SER
1	A	176	LYS
1	A	194	ASP
1	B	80	LYS
1	B	90	ARG
1	B	98	LYS
1	B	108	THR
1	B	114	ASN
1	B	122	THR
1	B	124	GLU

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Mol	Chain	Res	Type
1	B	125	LEU
1	B	127	SER
1	B	143	ASP
1	B	151	LYS
1	B	153	ARG
1	B	164	ARG
1	B	174	GLN
1	B	178	ILE
1	B	190	LEU
1	B	194	ASP
1	C	101	ASN
1	C	120	ARG
1	C	122	THR
1	C	143	ASP
1	C	153	ARG
1	C	172	ASN
1	C	194	ASP
1	D	108	THR
1	D	114	ASN
1	D	116	PHE
1	D	126	LYS
1	D	143	ASP
1	D	153	ARG
1	D	194	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	ASN
1	A	101	ASN
1	A	114	ASN
1	A	132	HIS
1	A	139	GLN
1	A	177	GLN
1	B	132	HIS
1	B	139	GLN
1	B	174	GLN
1	B	177	GLN
1	C	78	ASN
1	C	101	ASN
1	C	114	ASN
1	C	132	HIS

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Mol	Chain	Res	Type
1	C	139	GLN
1	D	114	ASN
1	D	132	HIS
1	D	139	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

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, 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	114/124 (91%)	0.26	6 (5%) 26 32	18, 31, 57, 71	0
1	B	114/124 (91%)	0.69	14 (12%) 4 5	18, 36, 78, 85	0
1	C	116/124 (93%)	0.37	8 (6%) 16 21	17, 30, 56, 72	0
1	D	113/124 (91%)	0.52	12 (10%) 6 7	16, 31, 75, 82	0
2	Q	25/35 (71%)	0.34	3 (12%) 4 5	29, 41, 116, 123	0
2	R	25/35 (71%)	0.31	3 (12%) 4 5	29, 43, 118, 162	0
All	All	507/566 (89%)	0.45	46 (9%) 9 12	16, 33, 73, 162	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	77	MET	6.8
1	D	116	PHE	6.5
1	B	125	LEU	5.9
1	B	117	TRP	5.6
1	D	125	LEU	5.4
1	A	173	SER	5.4
1	B	122	THR	5.0
1	B	118	ARG	4.8
1	D	117	TRP	4.6
1	C	168	THR	4.6
1	B	77	MET	4.6
2	Q	29	DT	4.6
2	R	13	DT	4.5
2	R	14	DT	4.4
1	C	172	ASN	4.3
1	D	168	THR	4.2
1	D	173	SER	4.2
1	B	186	ASN	4.1
1	B	123	ASN	4.1

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Mol	Chain	Res	Type	RSRZ
2	Q	13	DT	4.0
1	D	174	GLN	3.7
1	A	78	ASN	3.7
1	D	118	ARG	3.7
1	A	77	MET	3.7
1	D	119	ASP	3.7
2	Q	12	DT	3.6
2	R	12	DT	3.5
1	C	185	TYR	3.3
1	C	173	SER	3.2
1	A	167	HIS	3.1
1	B	169	ASN	3.1
1	A	174	GLN	3.0
1	B	119	ASP	2.9
1	B	168	THR	2.9
1	C	78	ASN	2.9
1	B	194	ASP	2.7
1	C	194	ASP	2.7
1	D	120	ARG	2.6
1	D	194	ASP	2.5
1	B	127	SER	2.4
1	D	124	GLU	2.4
1	C	120	ARG	2.3
1	D	172	ASN	2.2
1	B	124	GLU	2.1
1	A	186	ASN	2.0
1	B	120	ARG	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

There are no such residues in this entry.