



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:53 PM UTC

PDB ID : 3ULP / pdb_00003ulp
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 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
Xtrriage (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

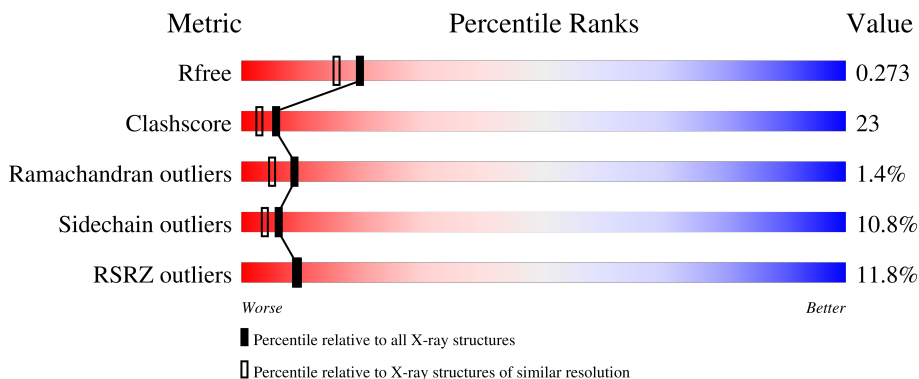
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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.



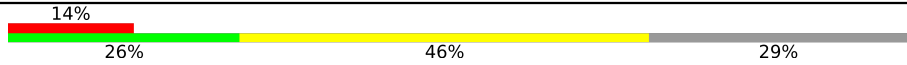
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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 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	124	 6% 64% 26% 8%
1	B	124	 13% 58% 26% 6% 8%
1	C	124	 7% 59% 30% 5% 6%
1	D	124	 14% 55% 27% 8% 9%
2	Q	35	 17% 34% 34% 29%

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Mol	Chain	Length	Quality of chain
2	R	35	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a red segment (14%), a green segment (26%), a yellow segment (46%), and a grey segment (14%). The percentages are labeled below each segment.</p>

2 Entry composition [i](#)

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
			Total	C	N	O	S			
1	A	114	Total 918	C 580	N 168	O 168	S 2	0	0	0
1	B	114	Total 898	C 568	N 161	O 167	S 2	0	0	0
1	C	116	Total 936	C 592	N 171	O 171	S 2	0	0	0
1	D	113	Total 886	C 566	N 159	O 159	S 2	0	0	0

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

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

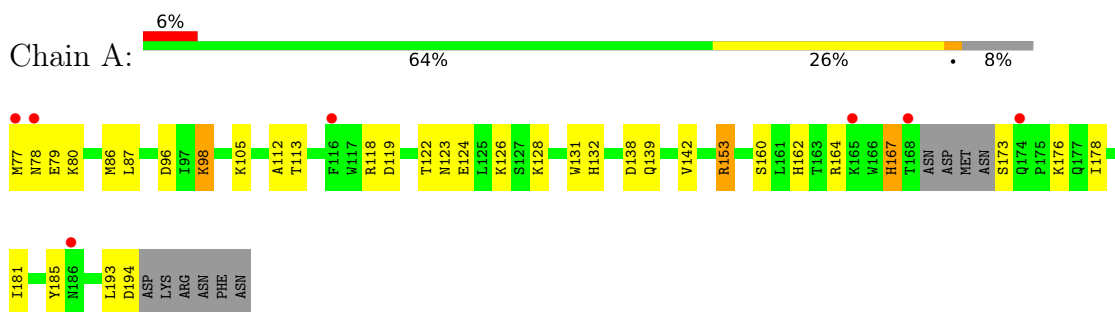
- Molecule 3 is water.

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

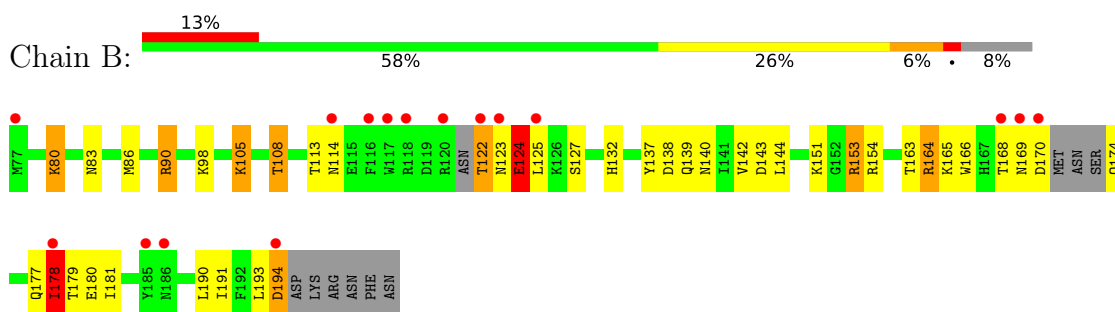
3 Residue-property plots [i](#)

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.

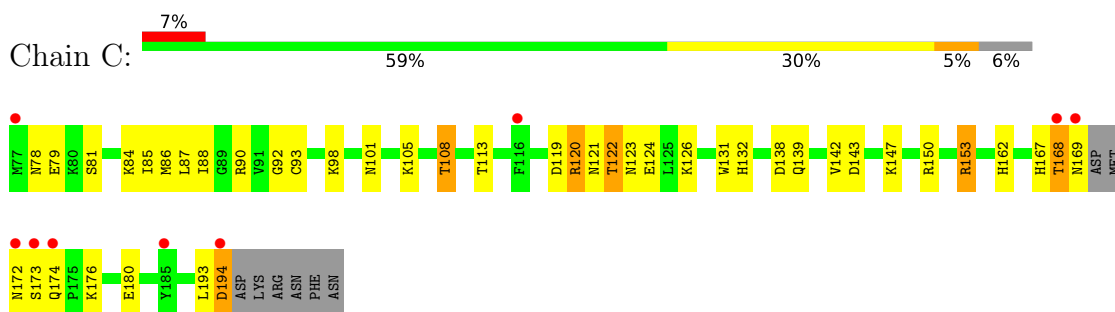
- Molecule 1: Single-strand binding protein



- Molecule 1: Single-strand binding protein

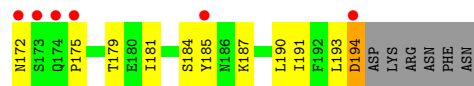


- Molecule 1: Single-strand binding protein

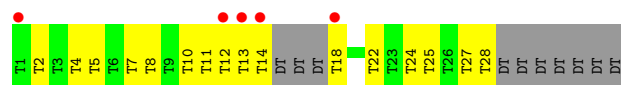


- Molecule 1: Single-strand binding protein

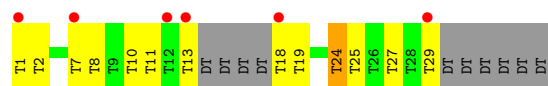




- Molecule 2: DNA (35-MER)



- 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 30.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.2 (30.00-2.10) 99.2 (30.00-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.88 (at 2.10Å)	Xtrriage
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 (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	33.1	Xtrriage
Anisotropy	0.400	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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 [i](#)

5.1 Standard geometry [i](#)

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	0.61	0/932	0.88	0/1255
1	B	0.56	0/911	0.83	1/1228 (0.1%)
1	C	0.61	0/951	0.87	0/1281
1	D	0.64	0/900	0.88	1/1211 (0.1%)
2	Q	0.34	0/548	1.14	1/842 (0.1%)
2	R	0.31	0/570	1.08	0/876
All	All	0.55	0/4812	0.94	3/6693 (0.0%)

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 (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	178	ILE	CB-CA-C	-5.90	102.40	110.90
2	Q	24	DT	P-O3'-C3'	5.54	128.51	120.20
1	D	117	TRP	N-CA-C	5.02	115.93	108.60

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	918	0	926	31	1
1	B	898	0	881	46	0
1	C	936	0	936	69	1
1	D	886	0	875	54	0
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	207	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 (207) 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:H71	3:R:239:HOH:O	1.30	1.30
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:ARG:CG	1:B:153:ARG:HH11	1.61	1.12
1:A:153:ARG:HG2	1:A:153:ARG:NH1	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:HH11	1:B:153:ARG:HG3	1.33	0.92
1:B:163:THR:CG2	1:B:179:THR:HG22	1.98	0.92
1:B:153:ARG:HH11	1:B:153:ARG:HG2	1.34	0.92
1:C:105:LYS:H	1:C:139:GLN:HE22	1.11	0.91
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:D:77:MET:C	2:Q:11:DT:H71	1.95	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: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:C:193:LEU:C	1:C:194:ASP:OD1	2.21	0.84
1:A:105:LYS:H	1:A:139:GLN:HE22	1.22	0.82
1:C:153:ARG:CG	1:C:153:ARG:HH11	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:HH11	1:D:153:ARG:CG	1.95	0.79
1:C:113:THR:HG23	3:D:214:HOH:O	1.82	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:A:86:MET:SD	1:D:86:MET:HE1	2.23	0.78
1:D:78:ASN:HA	2:Q:11:DT:C7	2.14	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:164:ARG:NH1	1:B:178:ILE:HD11	1.99	0.77
2:Q:29:DT:C6	2:Q:29:DT:H5''	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:HH11	1:C:153:ARG:HG2	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:HH11	1:D:153:ARG:HG2	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
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:C:84:LYS:HD2	1:C:86:MET:HE2	1.77	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:B:86:MET:HE1	1:C:86:MET:SD	2.38	0.64
1:C:153:ARG:HH11	1:C:153:ARG:CB	2.11	0.63
1:D:193:LEU:O	1:D:194:ASP:CG	2.41	0.63
1:D:153:ARG:HG2	1:D:153:ARG:NH1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:R:18[A]:DT:C7	3:R:239:HOH:O	2.07	0.61
1:B:122:THR:C	1:B:124:GLU:H	2.09	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:84:LYS:CD	1:C:86:MET:HE2	2.32	0.59
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: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:CG	1:A:153:ARG:NH1	2.31	0.58
1:B:90:ARG:CZ	2:R:27:DT:H4'	2.34	0.58
1:C:119:ASP:HB3	1:C:122:THR:HG22	1.86	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
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:143:ASP:CG	3:D:207:HOH:O	2.49	0.53
1:C:88:ILE:O	1:D:81:SER:HB2	2.08	0.53
1:D:153:ARG:HH11	1:D:153:ARG:HB3	1.73	0.53
1:D:161:LEU:HD11	1:D:179:THR:CG2	2.39	0.53
1:B:191:ILE:HG12	1:D:80:LYS:HD2	1.90	0.53
1:D:123:ASN:O	1:D:124:GLU:O	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:81:SER:HB2	1:D:88:ILE:O	2.15	0.47
1:C:93:CYS:SG	3:Q:69:HOH:O	2.20	0.47
1:B:140:ASN:CG	3:B:207:HOH:O	2.57	0.47
1:B:169:ASN:O	1:B:170:ASP:C	2.57	0.47
1:B:168:THR:O	1:B:169:ASN:C	2.58	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
1:D:194:ASP:OD2	1:D:194:ASP:C	2.58	0.46
2:Q:1:DT:C2'	2:Q:2:DT:OP2	2.63	0.46
1:B:193:LEU:O	1:B:194:ASP:CG	2.59	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
1:A:193:LEU:O	1:A:194:ASP:C	2.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:181:ILE:HD12	1:B:181:ILE:N	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:B:122:THR:C	1:B:124:GLU:N	2.75	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:D:184:SER:O	1:D:185:TYR:C	2.61	0.42
1:A:178:ILE:HD12	2:R:5:DT:H2''	2.02	0.41
1:C:119:ASP:HB3	1:C:122:THR:CG2	2.50	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:B:165:LYS:HZ3	1:B:177:GLN:NE2	2.17	0.41
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:86:MET:HE1	1:D:86:MET:SD	2.61	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: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:B:144:LEU:HD13	2:Q:13:DT:H3'	2.02	0.40
1:C:162:HIS:HE1	1:D:115:GLU:HG3	1.83	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 [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	110/124 (89%)	107 (97%)	3 (3%)	0	100	100
1	B	108/124 (87%)	103 (95%)	4 (4%)	1 (1%)	14	10
1	C	112/124 (90%)	108 (96%)	2 (2%)	2 (2%)	6	3
1	D	107/124 (86%)	100 (94%)	4 (4%)	3 (3%)	4	1
All	All	437/496 (88%)	418 (96%)	13 (3%)	6 (1%)	9	5

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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	100/115 (87%)	94 (94%)	6 (6%)	17	15
1	B	95/115 (83%)	77 (81%)	18 (19%)	1	1
1	C	101/115 (88%)	93 (92%)	8 (8%)	11	9
1	D	92/115 (80%)	82 (89%)	10 (11%)	6	4
All	All	388/460 (84%)	346 (89%)	42 (11%)	6	4

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	LYS
1	A	98	LYS
1	A	153	ARG
1	A	167	HIS
1	A	173	SER
1	A	176	LYS
1	B	80	LYS
1	B	90	ARG
1	B	98	LYS
1	B	105	LYS
1	B	108	THR
1	B	114	ASN
1	B	122	THR
1	B	124	GLU
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	108	THR
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	80	LYS

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Mol	Chain	Res	Type
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	181	ILE
1	D	190	LEU
1	D	194	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	ASN
1	A	101	ASN
1	A	132	HIS
1	A	139	GLN
1	A	177	GLN
1	B	132	HIS
1	B	139	GLN
1	B	167	HIS
1	B	174	GLN
1	B	177	GLN
1	C	78	ASN
1	C	101	ASN
1	C	132	HIS
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 oligosaccharides 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%)	0.14	7 (6%) 27 29	18, 31, 57, 71	0
1	B	114/124 (91%)	0.62	16 (14%) 6 6	18, 36, 78, 85	0
1	C	116/124 (93%)	0.21	9 (7%) 19 20	17, 30, 56, 72	0
1	D	113/124 (91%)	0.44	17 (15%) 5 5	16, 31, 75, 82	0
2	Q	25/35 (71%)	0.54	6 (24%) 2 2	29, 41, 116, 123	0
2	R	25/35 (71%)	0.59	5 (20%) 3 3	22, 43, 118, 162	1 (4%)
All	All	507/566 (89%)	0.37	60 (11%) 9 9	16, 33, 73, 162	1 (0%)

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Q	13	DT	5.4
1	D	116	PHE	5.3
1	B	194	ASP	4.8
1	D	123	ASN	4.8
1	B	170	ASP	4.5
2	R	14	DT	4.4
1	C	194	ASP	4.4
1	B	117	TRP	4.3
1	B	116	PHE	4.2
1	D	173	SER	4.1
1	B	125	LEU	4.0
1	D	172	ASN	4.0
1	D	194	ASP	3.7
1	D	117	TRP	3.7
1	D	174	GLN	3.7
2	Q	12	DT	3.6
1	D	175	PRO	3.6
1	B	120	ARG	3.6
1	D	118	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	120	ARG	3.5
1	B	169	ASN	3.5
2	R	13	DT	3.5
1	B	77	MET	3.4
1	B	186	ASN	3.4
1	C	172	ASN	3.4
2	R	12	DT	3.4
1	A	77	MET	3.3
1	B	118	ARG	3.3
2	R	18[A]	DT	3.2
1	A	174	GLN	3.1
1	B	123	ASN	3.0
1	D	119	ASP	3.0
1	B	122	THR	3.0
1	C	185	TYR	3.0
1	D	125	LEU	2.8
1	C	116	PHE	2.8
1	D	77	MET	2.7
1	D	168	THR	2.6
1	C	77	MET	2.5
1	C	173	SER	2.5
1	A	116	PHE	2.5
1	B	185	TYR	2.4
1	D	185	TYR	2.4
1	C	168	THR	2.4
1	B	114	ASN	2.3
2	R	1	DT	2.3
1	C	174	GLN	2.2
1	D	127	SER	2.2
1	A	186	ASN	2.2
1	C	169	ASN	2.2
2	Q	18	DT	2.2
2	Q	29	DT	2.2
2	Q	1	DT	2.2
1	B	178	ILE	2.1
1	A	168	THR	2.1
1	A	78	ASN	2.1
1	B	168	THR	2.0
1	A	165	LYS	2.0
2	Q	7	DT	2.0
1	D	96	ASP	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.