



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 03:15 am BST

PDB ID : 5X7V  
Title : Crystal structure of Nucleosome assembly protein S (PfNapS) from Plasmodium falciparum  
Authors : Gill, J.; Yogavel, M.; Sharma, A.  
Deposited on : 2017-02-27  
Resolution : 2.80 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](mailto: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.

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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

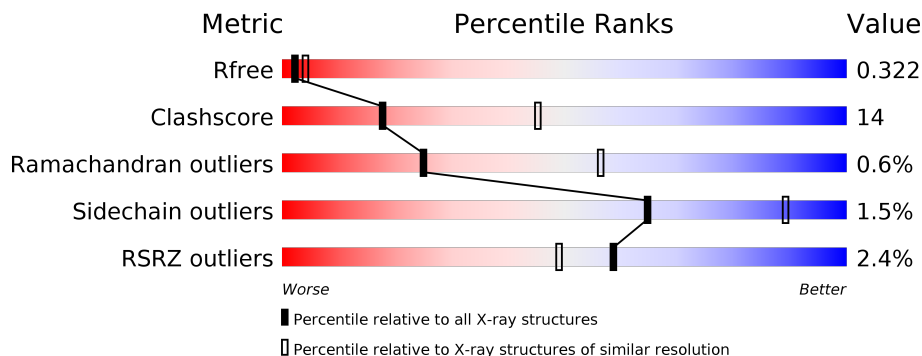
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 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	193	
1	B	193	
1	C	193	
1	D	193	
1	E	193	
1	F	193	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8441 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.

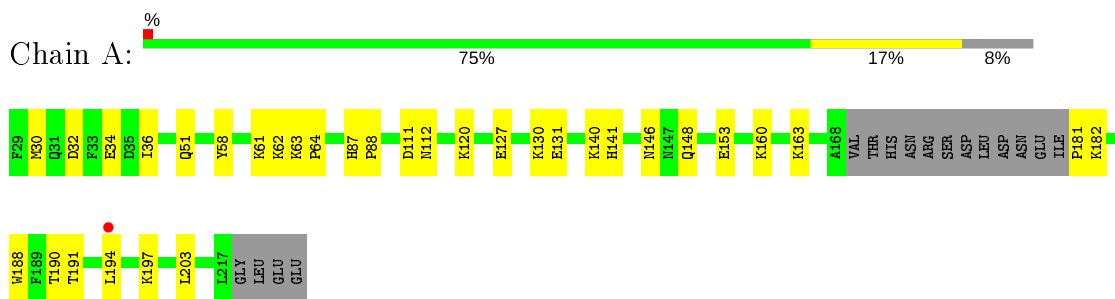
- Molecule 1 is a protein called Nucleosome assembly protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	177	1467	948	242	271	6	0	0	0
1	B	160	1330	862	219	244	5	0	0	0
1	C	179	1450	943	240	261	6	0	0	0
1	D	172	1437	931	238	262	6	0	0	0
1	E	167	1377	893	226	252	6	0	0	0
1	F	168	1380	896	228	250	6	0	0	0

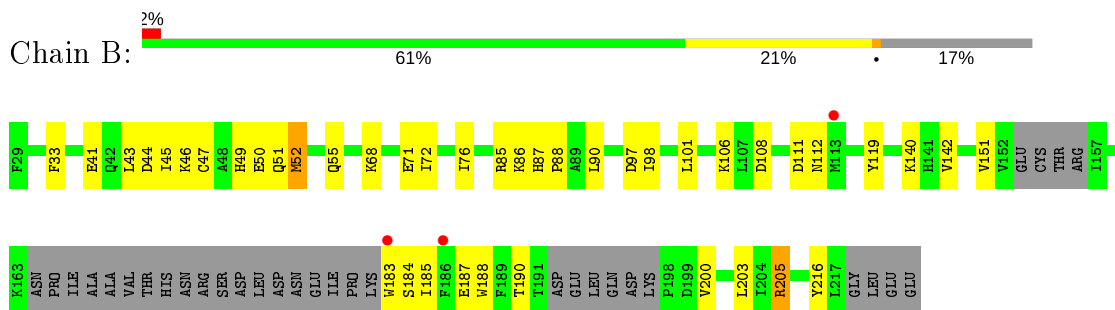
### 3 Residue-property plots [i](#)

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

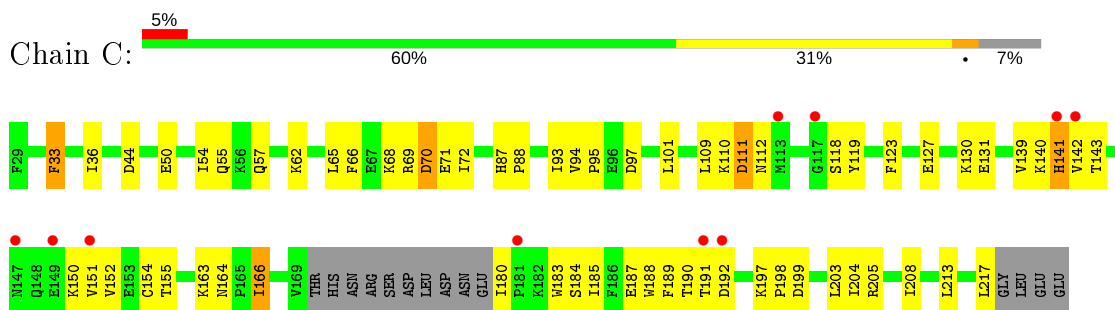
- Molecule 1: Nucleosome assembly protein



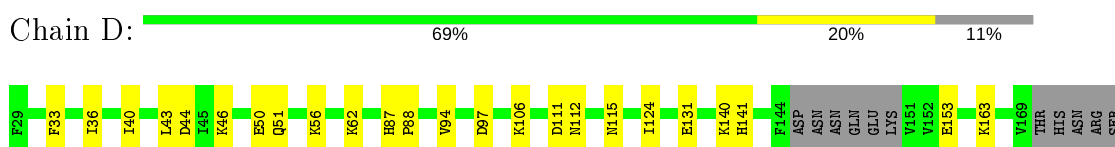
- Molecule 1: Nucleosome assembly protein



- Molecule 1: Nucleosome assembly protein



- Molecule 1: Nucleosome assembly protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	95.79Å 114.90Å 139.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.24 – 2.80 44.29 – 2.80	Depositor EDS
% Data completeness (in resolution range)	89.1 (29.24-2.80) 91.2 (44.29-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.82 (at 2.81Å)	Xtrriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, $R_{free}$	0.243 , 0.312 0.259 , 0.322	Depositor DCC
$R_{free}$ test set	1752 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	14.3	Xtrriage
Anisotropy	2.267	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 38.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	8441	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical 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	0.52	0/1502	0.63	0/2026
1	B	0.59	0/1361	0.68	0/1834
1	C	0.58	0/1485	0.68	0/2007
1	D	0.60	0/1471	0.69	0/1983
1	E	0.55	0/1409	0.65	0/1900
1	F	0.57	0/1412	0.70	0/1903
All	All	0.57	0/8640	0.67	0/11653

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	1467	0	1440	29	0
1	B	1330	0	1287	44	0
1	C	1450	0	1419	59	0
1	D	1437	0	1426	33	0
1	E	1377	0	1356	42	0
1	F	1380	0	1347	49	0
All	All	8441	0	8275	228	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 14.

All (228) 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:F:133:MET:CE	1:F:159:TRP:CZ3	2.18	1.26
1:F:133:MET:HE3	1:F:159:TRP:HZ3	1.21	1.05
1:F:133:MET:HE3	1:F:159:TRP:CZ3	1.93	1.02
1:F:133:MET:CE	1:F:159:TRP:HZ3	1.64	0.97
1:E:30:MET:CE	1:F:217:LEU:HD21	1.96	0.95
1:A:51:GLN:O	1:B:51:GLN:NE2	2.01	0.93
1:F:133:MET:HE2	1:F:159:TRP:CZ3	2.06	0.89
1:E:30:MET:HE1	1:F:217:LEU:HD21	1.57	0.84
1:C:150:LYS:O	1:C:151:VAL:HG23	1.81	0.81
1:C:164:ASN:OD1	1:C:166:ILE:HG13	1.81	0.81
1:B:87:HIS:HD2	1:B:88:PRO:HD2	1.46	0.79
1:C:69:ARG:O	1:C:71:GLU:N	2.16	0.78
1:B:90:LEU:CD2	1:B:183:TRP:HH2	1.97	0.77
1:C:101:LEU:HD11	1:C:185:ILE:CD1	2.16	0.76
1:C:164:ASN:OD1	1:C:166:ILE:CG1	2.34	0.75
1:F:36:ILE:O	1:F:40:ILE:HD12	1.87	0.73
1:C:101:LEU:HD11	1:C:185:ILE:HD12	1.69	0.73
1:F:133:MET:HE1	1:F:159:TRP:CZ3	2.23	0.73
1:F:206:ARG:HG2	1:F:206:ARG:O	1.88	0.72
1:C:154:CYS:SG	1:C:190:THR:N	2.62	0.72
1:D:87:HIS:HD2	1:D:88:PRO:HD2	1.55	0.72
1:D:195:GLN:O	1:D:195:GLN:HG3	1.90	0.72
1:C:150:LYS:O	1:C:151:VAL:CG2	2.38	0.71
1:F:34:GLU:O	1:F:38:LYS:HG2	1.90	0.71
1:A:181:PRO:O	1:A:182:LYS:HG3	1.91	0.70
1:D:87:HIS:HE1	1:D:203:LEU:HD22	1.56	0.70
1:E:30:MET:HE2	1:F:217:LEU:HD21	1.73	0.69
1:A:194:LEU:HD22	1:A:197:LYS:HD2	1.74	0.69
1:A:188:TRP:HD1	1:A:194:LEU:HD11	1.58	0.69
1:E:141:HIS:HB3	1:E:153:GLU:HB2	1.75	0.68
1:E:110:LYS:HG3	1:E:113:MET:HG3	1.75	0.68
1:E:103:HIS:CE1	1:E:128:LYS:HD2	2.29	0.68
1:B:140:LYS:HG2	1:B:188:TRP:CH2	2.29	0.68
1:C:87:HIS:HD2	1:C:88:PRO:HD2	1.58	0.68
1:C:139:VAL:HG22	1:C:155:THR:OG1	1.94	0.67
1:E:211:ASN:ND2	1:E:214:SER:OG	2.27	0.67
1:C:180:ILE:HD12	1:C:180:ILE:O	1.95	0.67
1:B:52:MET:O	1:B:55:GLN:N	2.28	0.67
1:B:97:ASP:OD2	1:B:185:ILE:N	2.26	0.66
1:C:213:LEU:HD22	1:D:33:PHE:HB3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:TYR:CE2	1:B:205:ARG:HD3	2.32	0.65
1:C:142:VAL:HG22	1:C:152:VAL:HG22	1.80	0.64
1:A:141:HIS:HB3	1:A:153:GLU:HB2	1.81	0.63
1:A:188:TRP:CD1	1:A:194:LEU:HD11	2.33	0.63
1:C:69:ARG:O	1:C:70:ASP:C	2.35	0.63
1:A:61:LYS:HB3	1:B:43:LEU:HD21	1.80	0.62
1:F:109:LEU:O	1:F:111:ASP:N	2.32	0.62
1:A:32:ASP:HB3	1:B:72:ILE:CD1	2.30	0.61
1:F:159:TRP:NE1	1:F:164:ASN:OD1	2.34	0.61
1:B:87:HIS:CD2	1:B:88:PRO:HD2	2.32	0.61
1:F:88:PRO:HG2	1:F:203:LEU:HD22	1.82	0.61
1:C:111:ASP:OD1	1:C:111:ASP:N	2.24	0.61
1:A:32:ASP:HB3	1:B:72:ILE:HD11	1.83	0.60
1:A:32:ASP:O	1:A:36:ILE:HG12	2.01	0.60
1:B:46:LYS:O	1:B:47:CYS:C	2.39	0.60
1:B:183:TRP:HZ3	1:B:185:ILE:HA	1.67	0.59
1:F:140:LYS:HG2	1:F:188:TRP:CH2	2.38	0.59
1:A:127:GLU:OE2	1:A:130:LYS:NZ	2.36	0.58
1:F:143:THR:O	1:F:150:LYS:HA	2.04	0.58
1:E:39:ASP:O	1:E:43:LEU:HD23	2.04	0.58
1:E:68:LYS:HB3	1:F:36:ILE:HD11	1.85	0.58
1:F:152:VAL:HG13	1:F:152:VAL:O	2.04	0.57
1:F:159:TRP:CD1	1:F:164:ASN:OD1	2.57	0.57
1:C:87:HIS:HE1	1:C:203:LEU:HD22	1.69	0.57
1:C:93:ILE:HD13	1:C:185:ILE:HD11	1.86	0.57
1:C:187:GLU:OE1	1:C:197:LYS:HE2	2.04	0.57
1:E:199:ASP:HB3	1:E:202:GLU:HB2	1.87	0.56
1:F:109:LEU:CD2	1:F:205:ARG:HA	2.35	0.56
1:F:144:PHE:CE1	1:F:150:LYS:HB2	2.41	0.56
1:F:109:LEU:HD22	1:F:205:ARG:HA	1.87	0.55
1:F:144:PHE:CE1	1:F:150:LYS:CB	2.89	0.55
1:B:119:TYR:CD2	1:B:205:ARG:HD2	2.42	0.55
1:A:181:PRO:O	1:A:182:LYS:CG	2.54	0.55
1:C:164:ASN:OD1	1:C:166:ILE:HG12	2.05	0.55
1:F:184:SER:O	1:F:187:GLU:HB2	2.06	0.55
1:C:150:LYS:C	1:C:151:VAL:HG23	2.25	0.55
1:C:54:ILE:HD13	1:C:57:GLN:NE2	2.23	0.54
1:D:106:LYS:HD2	1:D:124:ILE:HD12	1.89	0.54
1:E:111:ASP:OD1	1:E:112:ASN:N	2.39	0.54
1:A:61:LYS:O	1:A:64:PRO:HD2	2.06	0.54
1:E:200:VAL:O	1:E:204:ILE:HD12	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:GLU:O	1:C:163:LYS:HG3	2.09	0.53
1:E:131:GLU:OE2	1:E:163:LYS:NZ	2.42	0.53
1:F:112:ASN:OD1	1:F:113:MET:N	2.41	0.53
1:E:140:LYS:HD3	1:E:188:TRP:CH2	2.43	0.53
1:B:183:TRP:HE3	1:B:184:SER:O	1.91	0.53
1:C:87:HIS:CD2	1:C:88:PRO:HD2	2.42	0.53
1:B:90:LEU:HD22	1:B:183:TRP:HH2	1.73	0.53
1:C:50:GLU:O	1:C:54:ILE:HG12	2.08	0.53
1:E:213:LEU:HB2	1:F:33:PHE:CE2	2.43	0.53
1:A:62:LYS:NZ	1:B:44:ASP:OD1	2.31	0.53
1:C:69:ARG:C	1:C:71:GLU:N	2.61	0.53
1:D:111:ASP:OD1	1:D:112:ASN:N	2.42	0.52
1:D:140:LYS:HD3	1:D:188:TRP:CZ2	2.45	0.52
1:C:62:LYS:NZ	1:D:44:ASP:OD1	2.30	0.52
1:B:142:VAL:HG22	1:B:151:VAL:HG23	1.90	0.52
1:B:90:LEU:CD2	1:B:183:TRP:CH2	2.85	0.52
1:C:44:ASP:OD1	1:D:62:LYS:NZ	2.26	0.52
1:B:119:TYR:CD2	1:B:205:ARG:CD	2.93	0.52
1:A:111:ASP:OD1	1:A:112:ASN:N	2.42	0.52
1:C:127:GLU:O	1:C:130:LYS:HG3	2.10	0.52
1:A:131:GLU:HG2	1:A:163:LYS:HE3	1.92	0.51
1:B:87:HIS:HE1	1:B:203:LEU:HD22	1.75	0.51
1:E:107:LEU:O	1:E:209:TRP:HZ3	1.92	0.51
1:F:106:LYS:HB3	1:F:124:ILE:HB	1.92	0.51
1:B:119:TYR:CE2	1:B:205:ARG:CD	2.94	0.51
1:A:30:MET:O	1:A:34:GLU:HG3	2.10	0.50
1:B:90:LEU:HD23	1:B:183:TRP:CH2	2.46	0.50
1:C:55:GLN:HG2	1:D:51:GLN:HE22	1.77	0.50
1:B:183:TRP:HZ3	1:B:185:ILE:HD12	1.77	0.50
1:F:206:ARG:O	1:F:206:ARG:CG	2.58	0.50
1:A:120:LYS:HG3	1:A:141:HIS:HB2	1.93	0.50
1:E:202:GLU:OE1	1:E:205:ARG:NH2	2.44	0.49
1:F:79:PHE:HZ	1:F:212:PRO:HB2	1.77	0.49
1:B:111:ASP:OD1	1:B:112:ASN:N	2.41	0.49
1:E:100:ILE:HG21	1:E:133:MET:HE1	1.94	0.49
1:B:46:LYS:O	1:B:49:HIS:N	2.44	0.49
1:C:87:HIS:CE1	1:C:203:LEU:HD13	2.48	0.49
1:C:199:ASP:O	1:C:203:LEU:HG	2.12	0.49
1:F:140:LYS:HE3	1:F:154:CYS:HB2	1.94	0.49
1:E:130:LYS:HG3	1:E:136:LEU:HD11	1.94	0.48
1:E:103:HIS:HE1	1:E:128:LYS:HD2	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:105:VAL:HG12	1:F:124:ILE:O	2.12	0.48
1:D:202:GLU:OE1	1:D:206:ARG:NE	2.47	0.48
1:F:43:LEU:HA	1:F:43:LEU:HD23	1.60	0.48
1:C:140:LYS:HD3	1:C:188:TRP:CH2	2.49	0.48
1:F:144:PHE:CE1	1:F:150:LYS:HB3	2.49	0.48
1:D:194:LEU:O	1:D:194:LEU:HG	2.13	0.47
1:B:142:VAL:HG22	1:B:151:VAL:CG2	2.45	0.47
1:D:185:ILE:HG13	1:D:200:VAL:HG11	1.95	0.47
1:C:140:LYS:HD3	1:C:188:TRP:CZ2	2.50	0.47
1:E:82:ASN:O	1:E:86:LYS:HD2	2.15	0.47
1:C:213:LEU:HG	1:C:217:LEU:HD23	1.96	0.47
1:D:140:LYS:HD3	1:D:188:TRP:CH2	2.50	0.47
1:C:183:TRP:CZ2	1:C:198:PRO:HG2	2.50	0.47
1:F:82:ASN:OD1	1:F:85:ARG:NH1	2.48	0.47
1:D:188:TRP:CG	1:D:200:VAL:HG22	2.50	0.46
1:B:183:TRP:CZ3	1:B:185:ILE:HA	2.48	0.46
1:C:69:ARG:C	1:C:71:GLU:H	2.18	0.46
1:E:141:HIS:ND1	1:E:153:GLU:OE1	2.48	0.46
1:C:68:LYS:HB3	1:D:36:ILE:HD13	1.97	0.46
1:E:129:ALA:HB3	1:E:136:LEU:HD22	1.98	0.46
1:D:87:HIS:CD2	1:D:88:PRO:HD2	2.44	0.46
1:D:141:HIS:HB3	1:D:153:GLU:HB2	1.98	0.46
1:E:80:TRP:HB3	1:E:104:LEU:HD23	1.97	0.46
1:F:68:LYS:HA	1:F:68:LYS:HD2	1.79	0.46
1:C:123:PHE:CD1	1:C:189:PHE:HZ	2.34	0.46
1:D:197:LYS:HB3	1:D:198:PRO:HD2	1.98	0.46
1:C:112:ASN:N	1:C:118:SER:O	2.49	0.46
1:C:213:LEU:HG	1:C:217:LEU:CD2	2.46	0.45
1:A:87:HIS:ND1	1:A:88:PRO:HD2	2.30	0.45
1:A:32:ASP:CB	1:B:72:ILE:HD13	2.46	0.45
1:A:63:LYS:HB2	1:A:64:PRO:HD3	1.97	0.45
1:E:211:ASN:HA	1:F:37:GLN:NE2	2.31	0.45
1:C:110:LYS:O	1:C:119:TYR:HA	2.17	0.45
1:C:101:LEU:CD1	1:C:185:ILE:HD12	2.43	0.45
1:C:69:ARG:O	1:C:72:ILE:N	2.50	0.45
1:E:72:ILE:O	1:E:76:ILE:HD12	2.16	0.45
1:B:43:LEU:HA	1:B:43:LEU:HD12	1.82	0.45
1:D:193:GLU:N	1:D:193:GLU:OE1	2.50	0.45
1:E:212:PRO:HG2	1:F:33:PHE:HZ	1.81	0.45
1:A:146:ASN:C	1:A:148:GLN:H	2.20	0.45
1:D:94:VAL:O	1:D:97:ASP:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:LYS:HE2	1:B:108:ASP:OD2	2.17	0.44
1:C:44:ASP:OD2	1:D:210:HIS:NE2	2.50	0.44
1:B:76:ILE:O	1:B:76:ILE:HG22	2.18	0.44
1:D:197:LYS:HB3	1:D:198:PRO:CD	2.48	0.44
1:C:213:LEU:HD13	1:D:33:PHE:CG	2.53	0.44
1:E:62:LYS:HA	1:E:65:LEU:HD23	1.97	0.44
1:C:33:PHE:O	1:C:36:ILE:HG22	2.18	0.44
1:E:160:LYS:O	1:E:161:GLU:C	2.55	0.44
1:C:139:VAL:CG2	1:C:155:THR:OG1	2.62	0.44
1:E:211:ASN:OD1	1:F:37:GLN:NE2	2.46	0.44
1:A:87:HIS:HE2	1:A:203:LEU:HD22	1.83	0.44
1:E:36:ILE:O	1:E:40:ILE:HG12	2.18	0.44
1:F:119:TYR:CD1	1:F:205:ARG:HD3	2.53	0.44
1:A:190:THR:OG1	1:A:191:THR:N	2.51	0.44
1:D:192:ASP:C	1:D:192:ASP:OD1	2.56	0.44
1:D:56:LYS:NZ	1:D:115:ASN:OD1	2.36	0.43
1:D:87:HIS:CE1	1:D:203:LEU:HD22	2.45	0.43
1:D:46:LYS:O	1:D:50:GLU:HG3	2.18	0.43
1:F:35:ASP:O	1:F:38:LYS:HB2	2.17	0.43
1:F:133:MET:CE	1:F:159:TRP:CH2	2.90	0.43
1:C:65:LEU:HD23	1:C:65:LEU:HA	1.82	0.43
1:B:200:VAL:HA	1:B:203:LEU:HD12	2.01	0.43
1:C:109:LEU:HD22	1:C:205:ARG:HA	2.01	0.43
1:C:62:LYS:HG3	1:D:43:LEU:CD2	2.48	0.43
1:A:130:LYS:O	1:A:160:LYS:NZ	2.46	0.42
1:E:33:PHE:CG	1:F:213:LEU:HD13	2.54	0.42
1:B:142:VAL:HA	1:B:151:VAL:HG23	2.01	0.42
1:A:188:TRP:HD1	1:A:194:LEU:CD1	2.29	0.42
1:E:199:ASP:O	1:E:203:LEU:HG	2.19	0.42
1:C:164:ASN:CG	1:C:166:ILE:HG13	2.39	0.42
1:F:140:LYS:HG2	1:F:188:TRP:CZ2	2.54	0.42
1:C:204:ILE:HA	1:C:208:ILE:HB	2.00	0.42
1:C:183:TRP:CH2	1:C:198:PRO:HG2	2.55	0.42
1:E:143:THR:HB	1:E:151:VAL:HG12	2.01	0.42
1:C:97:ASP:OD2	1:C:184:SER:HA	2.19	0.42
1:C:55:GLN:HG2	1:D:51:GLN:NE2	2.35	0.42
1:B:86:LYS:HE2	1:B:216:TYR:O	2.20	0.42
1:C:191:THR:HG22	1:C:191:THR:O	2.20	0.42
1:B:101:LEU:HA	1:B:101:LEU:HD23	1.84	0.41
1:C:141:HIS:CE1	1:C:143:THR:HG22	2.55	0.41
1:B:68:LYS:O	1:B:72:ILE:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:131:GLU:HG2	1:E:163:LYS:HZ1	1.86	0.41
1:E:69:ARG:O	1:E:73:ILE:HG13	2.20	0.41
1:A:140:LYS:HD3	1:A:188:TRP:CZ2	2.56	0.41
1:A:32:ASP:HB3	1:B:72:ILE:HD13	2.03	0.41
1:B:187:GLU:O	1:B:190:THR:HG23	2.21	0.41
1:F:150:LYS:O	1:F:150:LYS:HG2	2.21	0.41
1:A:58:TYR:OH	1:B:50:GLU:OE2	2.35	0.41
1:B:90:LEU:HD22	1:B:185:ILE:HD13	2.02	0.41
1:D:131:GLU:O	1:D:163:LYS:HG3	2.20	0.41
1:E:115:ASN:HD22	1:E:115:ASN:HA	1.60	0.41
1:E:53:ASN:O	1:E:57:GLN:HG3	2.21	0.41
1:B:85:ARG:HD3	1:B:98:ILE:HD12	2.03	0.41
1:C:66:PHE:CE1	1:D:40:ILE:HD13	2.56	0.41
1:E:213:LEU:HB2	1:F:33:PHE:CD2	2.56	0.41
1:F:118:SER:HB3	1:F:143:THR:HA	2.03	0.41
1:D:185:ILE:HD13	1:D:185:ILE:HG21	1.88	0.41
1:E:109:LEU:HD23	1:E:209:TRP:CD1	2.56	0.41
1:B:45:ILE:O	1:B:46:LYS:C	2.54	0.40
1:F:203:LEU:HD12	1:F:203:LEU:C	2.41	0.40
1:E:152:VAL:HG12	1:E:153:GLU:N	2.36	0.40
1:E:92:ASP:N	1:E:92:ASP:OD1	2.52	0.40
1:B:41:GLU:O	1:B:44:ASP:HB2	2.20	0.40
1:F:60:GLU:O	1:F:63:LYS:HG2	2.21	0.40
1:C:94:VAL:HA	1:C:95:PRO:HD3	1.93	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	173/193 (90%)	163 (94%)	10 (6%)	0	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	152/193 (79%)	136 (90%)	16 (10%)	0	100	100
1	C	175/193 (91%)	156 (89%)	17 (10%)	2 (1%)	14	41
1	D	166/193 (86%)	156 (94%)	9 (5%)	1 (1%)	25	56
1	E	159/193 (82%)	147 (92%)	11 (7%)	1 (1%)	25	56
1	F	160/193 (83%)	151 (94%)	7 (4%)	2 (1%)	12	36
All	All	985/1158 (85%)	909 (92%)	70 (7%)	6 (1%)	25	56

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	110	LYS
1	C	70	ASP
1	C	192	ASP
1	D	199	ASP
1	E	154	CYS
1	F	151	VAL

### 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	159/181 (88%)	159 (100%)	0	100	100
1	B	143/181 (79%)	139 (97%)	4 (3%)	43	77
1	C	153/181 (84%)	149 (97%)	4 (3%)	46	79
1	D	158/181 (87%)	158 (100%)	0	100	100
1	E	150/181 (83%)	148 (99%)	2 (1%)	69	91
1	F	147/181 (81%)	143 (97%)	4 (3%)	44	78
All	All	910/1086 (84%)	896 (98%)	14 (2%)	65	89

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	33	PHE
1	B	52	MET
1	B	71	GLU
1	B	205	ARG
1	C	33	PHE
1	C	111	ASP
1	C	141	HIS
1	C	166	ILE
1	E	113	MET
1	E	183	TRP
1	F	30	MET
1	F	31	GLN
1	F	133	MET
1	F	157	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	146	ASN
1	B	53	ASN
1	B	87	HIS
1	B	103	HIS
1	C	57	GLN
1	C	87	HIS
1	D	51	GLN
1	D	87	HIS
1	E	103	HIS
1	E	115	ASN
1	E	211	ASN
1	F	37	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, 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	A	177/193 (91%)	0.03	1 (0%) 89 86	50, 57, 76, 85	0
1	B	160/193 (82%)	0.15	3 (1%) 66 59	53, 65, 86, 104	0
1	C	179/193 (92%)	0.31	10 (5%) 24 16	52, 62, 84, 95	0
1	D	172/193 (89%)	0.13	0 100 100	50, 59, 73, 88	0
1	E	167/193 (86%)	0.08	5 (2%) 50 40	54, 65, 82, 101	0
1	F	168/193 (87%)	0.15	6 (3%) 42 32	52, 64, 84, 94	0
All	All	1023/1158 (88%)	0.14	25 (2%) 59 49	50, 62, 82, 104	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	147	ASN	5.7
1	C	192	ASP	3.0
1	E	127	GLU	2.8
1	B	183	TRP	2.7
1	C	191	THR	2.7
1	B	186	PHE	2.7
1	C	181	PRO	2.7
1	E	116	ASN	2.7
1	C	117	GLY	2.7
1	A	194	LEU	2.6
1	F	57	GLN	2.6
1	F	110	LYS	2.4
1	C	151	VAL	2.4
1	C	141	HIS	2.4
1	C	149	GLU	2.4
1	E	117	GLY	2.3
1	E	162	GLY	2.2
1	F	58	TYR	2.2
1	F	54	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	113	MET	2.2
1	E	151	VAL	2.1
1	C	142	VAL	2.1
1	B	113	MET	2.1
1	F	88	PRO	2.0
1	F	152	VAL	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 [i](#)

There are no such residues in this entry.