



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:22 PM UTC

PDB ID : 4GCT / pdb_00004gct
Title : structure of No factor protein-DNA complex
Authors : Schumacher, M.A.
Deposited on : 2012-07-30
Resolution : 2.45 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

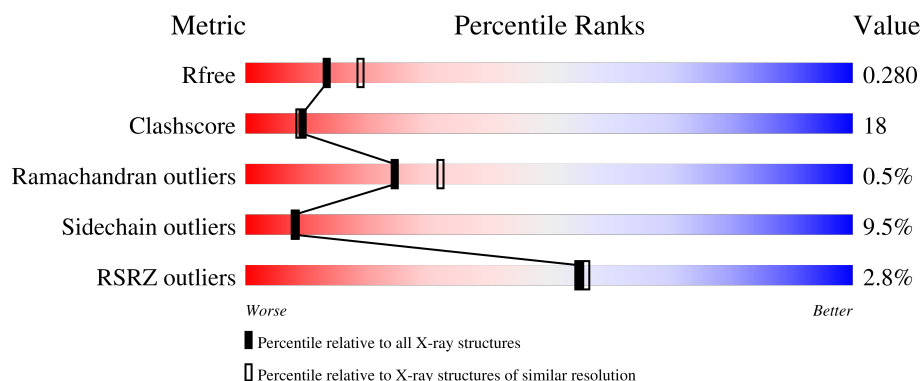
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	196	4% 62% 28% 6%
1	B	196	2% 59% 31% 6%
1	C	196	3% 61% 32% 6%
1	D	196	2% 57% 33% 7%
2	W	20	5% 40% 60%

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Mol	Chain	Length	Quality of chain
2	Z	20	5% 40% 55% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7196 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 Nucleoid occlusion factor SlmA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	185	Total	C	N	O	S	0	0	0
			1505	950	271	279	5			
1	B	189	Total	C	N	O	S	0	0	0
			1543	973	283	282	5			
1	C	190	Total	C	N	O	S	0	0	0
			1559	983	284	287	5			
1	D	189	Total	C	N	O	S	0	0	0
			1547	975	283	284	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	W	20	Total	C	N	O	P	0	0	0
			407	196	74	118	19			
2	Z	20	Total	C	N	O	P	0	0	0
			407	196	74	118	19			

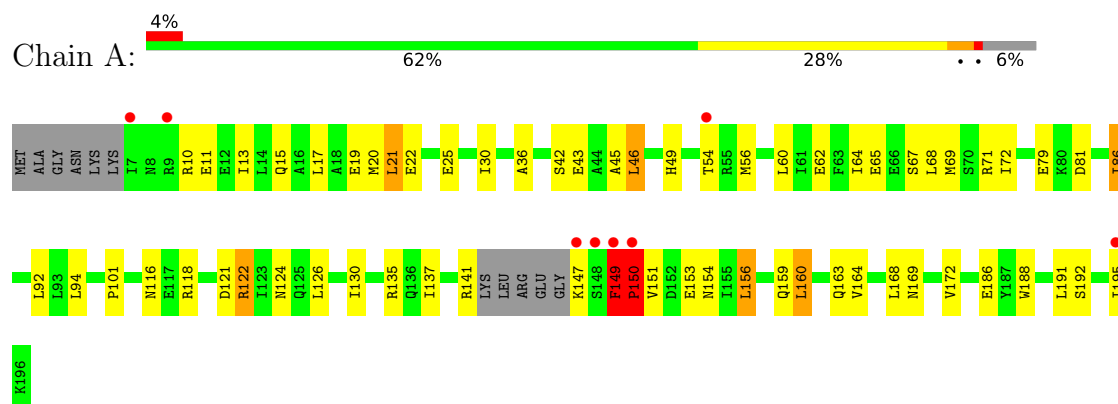
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	52	Total	O	0	0
			52	52		
3	B	51	Total	O	0	0
			51	51		
3	C	52	Total	O	0	0
			52	52		
3	D	46	Total	O	0	0
			46	46		
3	W	16	Total	O	0	0
			16	16		
3	Z	11	Total	O	0	0
			11	11		

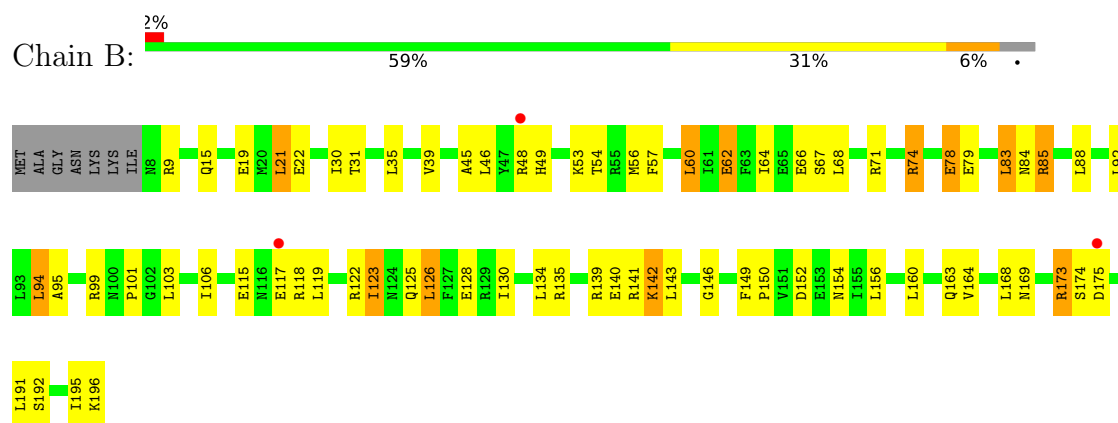
3 Residue-property plots [i](#)

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.

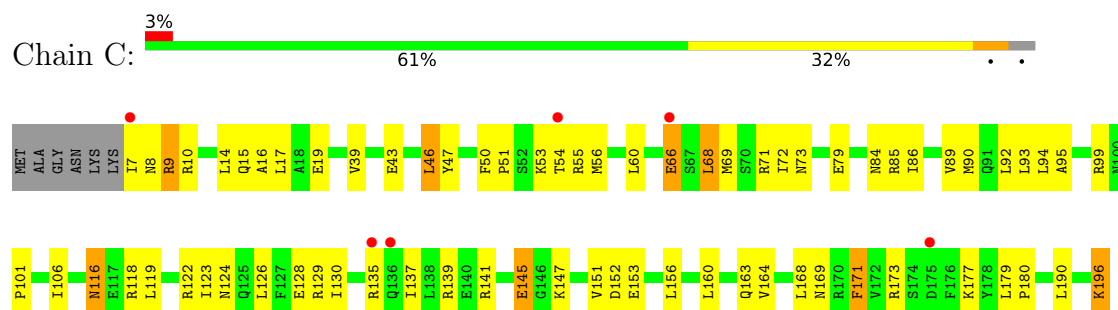
• Molecule 1: Nucleoid occlusion factor SlmA



• Molecule 1: Nucleoid occlusion factor SlmA

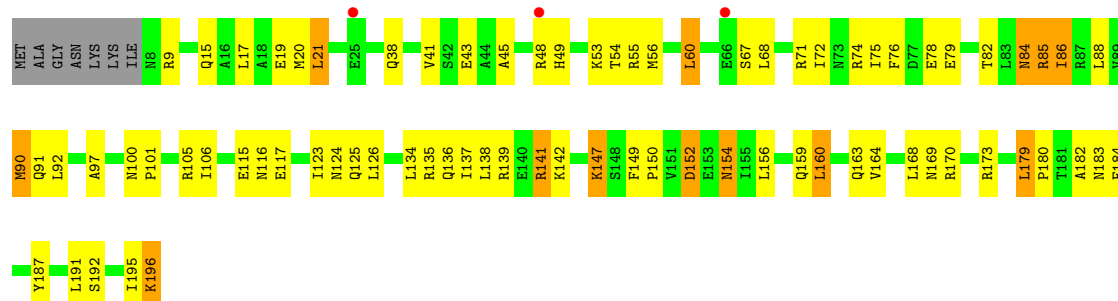


• Molecule 1: Nucleoid occlusion factor SlmA



- Molecule 1: Nucleoid occlusion factor SlmA

Chain D: 



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

Chain W: 



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

Chain Z: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	69.10Å 61.36Å 121.08Å 90.00° 99.06° 90.00°	Depositor
Resolution (Å)	63.75 – 2.45 63.75 – 2.45	Depositor EDS
% Data completeness (in resolution range)	90.7 (63.75-2.45) 90.8 (63.75-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 2.45Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.225 , 0.276 0.231 , 0.280	Depositor DCC
R_{free} test set	2678 reflections (7.91%)	wwPDB-VP
Wilson B-factor (Å ²)	48.9	Xtriage
Anisotropy	0.366	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 35.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7196	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.83 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2254e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.68	4/1525 (0.3%)	0.96	4/2046 (0.2%)
1	B	0.47	0/1564	0.87	1/2097 (0.0%)
1	C	0.47	0/1580	0.84	2/2118 (0.1%)
1	D	0.51	1/1568 (0.1%)	0.88	2/2102 (0.1%)
2	W	0.28	0/456	0.68	0/702
2	Z	0.36	0/456	0.73	0/702
All	All	0.51	5/7149 (0.1%)	0.86	9/9767 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	Z	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	149	PHE	CA-C	13.94	1.70	1.52
1	A	149	PHE	N-CA	8.65	1.58	1.46
1	A	150	PRO	N-CA	5.86	1.54	1.47
1	A	149	PHE	C-N	5.47	1.46	1.33
1	D	90	MET	SD-CE	5.43	1.93	1.79

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	150	PRO	CA-N-CD	-10.26	97.63	112.00
1	A	149	PHE	CB-CA-C	6.90	123.77	110.17
1	D	179	LEU	CA-C-N	6.79	126.59	119.05
1	D	179	LEU	C-N-CA	6.79	126.59	119.05
1	A	150	PRO	N-CA-CB	5.97	109.52	103.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	171	PHE	N-CA-C	-5.96	104.78	111.28
1	A	149	PHE	N-CA-CB	-5.75	100.14	110.37
1	B	78	GLU	N-CA-C	5.08	118.64	112.23
1	C	179	LEU	N-CA-C	5.06	116.89	109.71

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	Z	19	DT	Sidechain

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	1505	0	1518	46	0
1	B	1543	0	1573	59	0
1	C	1559	0	1592	69	0
1	D	1547	0	1577	62	0
2	W	407	0	228	15	0
2	Z	407	0	228	15	0
3	A	52	0	0	1	0
3	B	51	0	0	3	0
3	C	52	0	0	0	0
3	D	46	0	0	0	0
3	W	16	0	0	1	0
3	Z	11	0	0	0	0
All	All	7196	0	6716	246	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 18.

All (246) 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:B:53:LYS:HA	1:B:56:MET:HE3	1.29	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:MET:HE1	1:C:160:LEU:HB3	1.42	0.98
2:W:8:DA:H1'	2:W:9:DG:H5'	1.52	0.89
1:B:62:GLU:HG3	1:B:122:ARG:HH22	1.37	0.88
1:D:48:ARG:HH12	2:W:1:DT:H5'	1.34	0.88
2:W:4:DC:H1'	2:W:5:DG:H5'	1.56	0.87
1:B:54:THR:HG21	1:B:118:ARG:HD3	1.57	0.85
1:B:141:ARG:HH22	1:B:196:LYS:HA	1.41	0.85
1:B:15:GLN:O	1:B:19:GLU:HG3	1.78	0.83
1:C:79:GLU:O	1:C:85:ARG:HD3	1.80	0.81
1:D:48:ARG:NH1	2:W:1:DT:H5'	1.95	0.81
1:C:163:GLN:NE2	1:D:159:GLN:HG3	2.00	0.77
1:B:83:LEU:HD11	1:B:196:LYS:HG2	1.68	0.76
1:B:62:GLU:HG3	1:B:122:ARG:NH2	2.01	0.76
2:Z:20:DT:H2''	2:Z:21:DA:H5'	1.69	0.75
1:C:118:ARG:HH11	1:C:119:LEU:HD23	1.51	0.74
1:D:82:THR:HG21	1:D:141:ARG:HG3	1.70	0.74
1:C:54:THR:HG21	1:C:116:ASN:ND2	2.03	0.73
1:C:135:ARG:HH12	1:C:153:GLU:HB2	1.55	0.72
1:D:68:LEU:O	1:D:72:ILE:HG12	1.89	0.72
1:B:79:GLU:O	1:B:85:ARG:HD2	1.91	0.70
1:D:139:ARG:HG3	1:D:139:ARG:HH11	1.56	0.69
1:C:116:ASN:HB2	1:C:118:ARG:HG3	1.75	0.69
1:A:169:ASN:HD21	1:B:169:ASN:ND2	1.91	0.69
1:B:9:ARG:HG2	1:B:49:HIS:CE1	2.27	0.68
1:B:141:ARG:NH2	1:B:196:LYS:HA	2.09	0.68
1:C:86:ILE:HG13	1:C:137:ILE:HG21	1.77	0.67
1:B:48:ARG:HH22	2:Z:19:DT:H2'	1.60	0.67
2:Z:22:DC:H2''	2:Z:23:DG:O5'	1.94	0.67
1:A:69:MET:CE	1:A:130:ILE:HD13	2.25	0.66
1:A:163:GLN:NE2	1:B:163:GLN:HG2	2.11	0.66
1:B:48:ARG:NH2	2:Z:19:DT:H2'	2.10	0.66
1:A:149:PHE:O	1:A:151:VAL:HG23	1.96	0.65
1:D:182:ALA:O	1:D:183:ASN:HB2	1.97	0.65
1:D:20:MET:HE2	1:D:20:MET:HA	1.77	0.65
1:C:85:ARG:O	1:C:89:VAL:HG23	1.96	0.65
1:D:15:GLN:O	1:D:19:GLU:HG3	1.97	0.65
1:D:54:THR:HG21	1:D:116:ASN:HB2	1.79	0.65
1:C:106:ILE:HG22	1:C:123:ILE:HD11	1.79	0.64
2:Z:28:DT:H2''	2:Z:29:DA:C8	2.33	0.64
1:D:156:LEU:HD11	1:D:195:ILE:HD12	1.78	0.64
1:D:192:SER:O	1:D:196:LYS:HB2	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:ASN:ND2	1:B:169:ASN:ND2	2.46	0.63
1:C:141:ARG:HG2	1:C:147:LYS:HG3	1.77	0.63
1:C:124:ASN:O	1:C:128:GLU:HG2	2.00	0.62
1:D:20:MET:SD	1:D:38:GLN:HG3	2.40	0.62
1:A:22:GLU:HG3	1:A:101:PRO:HB2	1.81	0.61
1:B:169:ASN:O	1:B:173:ARG:HB2	2.01	0.60
1:D:135:ARG:HD3	1:D:154:ASN:ND2	2.17	0.60
1:C:145:GLU:O	1:C:147:LYS:HE3	2.02	0.60
1:A:71:ARG:HD2	1:A:92:LEU:HD11	1.83	0.60
1:D:17:LEU:O	1:D:21:LEU:HD22	2.02	0.59
1:A:54:THR:HG21	1:A:116:ASN:HB2	1.85	0.58
1:C:71:ARG:HD2	1:C:92:LEU:HD21	1.85	0.58
3:B:218:HOH:O	2:W:15:DA:H5''	2.03	0.58
2:Z:24:DT:H2''	2:Z:25:DG:N7	2.18	0.58
1:A:149:PHE:O	1:A:150:PRO:C	2.46	0.58
1:A:121:ASP:HB2	3:A:238:HOH:O	2.03	0.58
1:A:156:LEU:CD2	1:A:160:LEU:HD13	2.34	0.58
1:A:126:LEU:O	1:A:130:ILE:HG12	2.04	0.57
1:B:21:LEU:HD13	1:B:30:ILE:CD1	2.34	0.57
1:C:169:ASN:HD21	1:D:169:ASN:CG	2.13	0.56
1:D:91:GLN:HB2	1:D:184:PHE:CZ	2.41	0.56
1:C:151:VAL:HG22	1:C:152:ASP:N	2.21	0.56
1:D:139:ARG:HG3	1:D:139:ARG:NH1	2.20	0.56
1:B:141:ARG:HD2	1:B:149:PHE:CZ	2.41	0.55
1:D:9:ARG:HH11	1:D:41:VAL:HG11	1.71	0.55
1:C:118:ARG:HH11	1:C:119:LEU:CD2	2.19	0.55
1:D:79:GLU:HG2	1:D:84:ASN:HB3	1.88	0.55
1:D:139:ARG:NH2	1:D:154:ASN:HD21	2.04	0.54
1:C:151:VAL:HG22	1:C:152:ASP:H	1.71	0.54
1:C:90:MET:CE	1:C:160:LEU:HB3	2.27	0.54
1:C:71:ARG:CZ	1:C:99:ARG:NH2	2.71	0.54
1:B:74:ARG:HG2	1:B:78:GLU:OE2	2.07	0.54
1:C:51:PRO:HG2	1:C:55:ARG:HG3	1.89	0.53
1:B:149:PHE:HB3	1:B:150:PRO:HD2	1.91	0.53
1:C:90:MET:O	1:C:94:LEU:HD13	2.09	0.53
1:D:142:LYS:HA	1:D:147:LYS:O	2.08	0.53
1:B:71:ARG:HH11	1:B:92:LEU:HD11	1.73	0.53
1:A:10:ARG:HG3	1:A:49:HIS:HB3	1.90	0.53
1:B:135:ARG:O	1:B:139:ARG:HG3	2.08	0.53
1:D:9:ARG:HG2	1:D:9:ARG:HH21	1.74	0.53
1:A:69:MET:HE1	1:A:130:ILE:HD13	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:17:DG:H2'	2:W:18:DT:C6	2.44	0.52
1:A:65:GLU:HG2	1:A:126:LEU:HD13	1.92	0.52
1:D:139:ARG:HH21	1:D:154:ASN:HD21	1.58	0.52
2:W:8:DA:C1'	2:W:9:DG:H5'	2.34	0.52
1:A:156:LEU:HD22	1:A:160:LEU:HD13	1.92	0.52
1:B:71:ARG:HH11	1:B:71:ARG:HG3	1.74	0.52
1:B:84:ASN:O	1:B:88:LEU:HG	2.10	0.52
1:A:94:LEU:CD1	1:A:164:VAL:HG13	2.40	0.52
1:B:67:SER:O	1:B:71:ARG:HG3	2.09	0.52
1:C:141:ARG:O	1:C:145:GLU:HG3	2.09	0.51
1:D:71:ARG:HG2	1:D:71:ARG:HH11	1.76	0.51
1:C:106:ILE:CG2	1:C:123:ILE:HD11	2.39	0.51
1:C:135:ARG:HH11	1:C:135:ARG:HG2	1.76	0.51
1:C:7:ILE:HG22	1:C:8:ASN:N	2.26	0.51
1:A:192:SER:HA	1:A:195:ILE:HG22	1.93	0.51
1:B:57:PHE:CD2	1:B:115:GLU:HG2	2.46	0.51
2:W:4:DC:H1'	2:W:5:DG:C5'	2.37	0.51
1:A:135:ARG:HD3	1:A:154:ASN:HA	1.93	0.50
1:C:69:MET:HE3	1:C:126:LEU:CD1	2.40	0.50
2:Z:19:DT:H2''	2:Z:20:DT:OP2	2.10	0.50
1:A:65:GLU:OE2	1:A:122:ARG:NH1	2.44	0.50
1:A:69:MET:HE3	1:A:130:ILE:HD13	1.92	0.50
1:C:7:ILE:HB	1:C:10:ARG:HB3	1.93	0.50
2:W:10:DT:H5'	3:W:102:HOH:O	2.11	0.50
1:C:106:ILE:HG22	1:C:123:ILE:CD1	2.41	0.50
1:A:54:THR:CG2	1:A:116:ASN:HB2	2.41	0.50
1:A:69:MET:CE	1:A:72:ILE:HD12	2.42	0.50
1:C:15:GLN:O	1:C:19:GLU:HG3	2.12	0.49
1:C:141:ARG:HA	1:C:145:GLU:HG3	1.93	0.49
1:A:67:SER:O	1:A:71:ARG:HG3	2.12	0.49
1:D:170:ARG:HG2	1:D:173:ARG:HH21	1.76	0.49
1:A:69:MET:HE2	1:A:72:ILE:HD12	1.93	0.49
1:A:79:GLU:OE1	1:A:81:ASP:HB3	2.13	0.49
1:B:21:LEU:HD13	1:B:30:ILE:HD11	1.93	0.49
1:B:71:ARG:HG3	1:B:71:ARG:NH1	2.28	0.49
1:C:190:LEU:C	1:C:190:LEU:HD23	2.38	0.49
1:A:65:GLU:CG	1:A:126:LEU:HD13	2.42	0.49
1:C:190:LEU:HD23	1:C:190:LEU:O	2.13	0.49
1:B:54:THR:HG22	1:B:118:ARG:NH1	2.27	0.48
1:C:95:ALA:O	1:C:99:ARG:HG2	2.13	0.48
1:A:118:ARG:O	1:A:121:ASP:HB3	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:76:PHE:CZ	1:D:137:ILE:HG13	2.49	0.48
1:D:9:ARG:HG2	1:D:9:ARG:NH2	2.29	0.48
1:A:124:ASN:OD1	1:B:173:ARG:HD2	2.14	0.48
1:A:21:LEU:HD13	1:A:30:ILE:CD1	2.44	0.47
1:D:45:ALA:HA	1:D:48:ARG:HD2	1.97	0.47
1:A:36:ALA:HA	1:A:46:LEU:HD21	1.96	0.47
1:C:66:GLU:HA	1:C:66:GLU:OE1	2.13	0.47
1:C:93:LEU:HD21	1:C:130:ILE:CD1	2.44	0.47
1:D:67:SER:O	1:D:71:ARG:HG3	2.14	0.47
1:B:142:LYS:O	1:B:146:GLY:HA2	2.15	0.47
1:B:54:THR:CG2	1:B:118:ARG:HH11	2.28	0.47
2:Z:23:DG:H2'	2:Z:24:DT:C7	2.45	0.47
1:B:115:GLU:HB3	1:B:119:LEU:HD12	1.97	0.47
1:D:54:THR:CG2	1:D:116:ASN:HB2	2.44	0.47
1:B:94:LEU:CD1	1:B:164:VAL:HG22	2.45	0.47
1:C:164:VAL:O	1:C:168:LEU:HG	2.15	0.47
1:D:48:ARG:HG3	1:D:49:HIS:CE1	2.49	0.47
1:A:62:GLU:CG	1:A:122:ARG:HH22	2.28	0.47
1:B:9:ARG:HG2	1:B:49:HIS:NE2	2.29	0.47
1:D:179:LEU:HA	1:D:180:PRO:HD3	1.79	0.47
1:A:13:ILE:HG21	1:A:56:MET:HE2	1.97	0.46
1:D:86:ILE:O	1:D:90:MET:HG2	2.16	0.46
1:C:69:MET:SD	1:C:129:ARG:NH1	2.89	0.46
1:B:141:ARG:HH22	1:B:196:LYS:CA	2.18	0.46
1:C:43:GLU:O	1:C:46:LEU:HB2	2.16	0.46
1:D:75:ILE:HD13	1:D:88:LEU:HB3	1.98	0.46
1:C:93:LEU:HD11	1:C:130:ILE:HD13	1.97	0.46
1:D:149:PHE:HB3	1:D:150:PRO:HD2	1.98	0.46
1:D:156:LEU:CD2	1:D:160:LEU:HD22	2.45	0.46
1:A:141:ARG:O	1:A:147:LYS:HA	2.16	0.46
1:B:173:ARG:C	1:B:175:ASP:H	2.24	0.46
1:B:35:LEU:O	1:B:39:VAL:HG23	2.16	0.46
1:C:7:ILE:HG22	1:C:8:ASN:H	1.79	0.45
1:C:118:ARG:HD3	1:C:119:LEU:HD23	1.98	0.45
1:A:86:ILE:HG12	1:A:137:ILE:HG21	1.97	0.45
1:D:91:GLN:HB2	1:D:184:PHE:CE2	2.51	0.45
1:B:45:ALA:HA	1:B:48:ARG:NH1	2.31	0.45
1:B:31:THR:HG22	2:W:14:DC:H3'	1.97	0.45
1:B:64:ILE:HD11	1:B:103:LEU:HB3	1.99	0.45
1:B:169:ASN:HB2	3:B:227:HOH:O	2.15	0.45
1:D:152:ASP:OD1	1:D:154:ASN:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:60:LEU:HD23	1:D:106:ILE:HD11	1.99	0.45
1:D:48:ARG:NH1	2:W:1:DT:H6	2.16	0.44
1:D:60:LEU:HD23	1:D:106:ILE:CD1	2.47	0.44
2:Z:23:DG:H2'	2:Z:24:DT:C6	2.51	0.44
1:B:164:VAL:O	1:B:168:LEU:HG	2.17	0.44
1:A:60:LEU:O	1:A:64:ILE:HG13	2.18	0.44
1:A:168:LEU:O	1:A:172:VAL:HG23	2.17	0.44
1:D:45:ALA:O	1:D:48:ARG:HG2	2.18	0.44
1:C:16:ALA:CB	1:C:39:VAL:HG22	2.48	0.44
1:C:53:LYS:HE3	2:W:11:DA:OP1	2.17	0.44
1:B:117:GLU:O	1:B:118:ARG:C	2.61	0.44
1:C:47:TYR:HA	1:C:50:PHE:O	2.18	0.44
1:C:10:ARG:HG2	1:C:10:ARG:HH11	1.82	0.44
1:A:20:MET:HE3	1:A:25:GLU:OE1	2.18	0.44
1:C:51:PRO:CG	1:C:55:ARG:HG3	2.48	0.44
1:A:21:LEU:HD12	1:A:21:LEU:HA	1.86	0.43
1:B:126:LEU:O	1:B:130:ILE:HG13	2.18	0.43
1:B:54:THR:HG23	1:B:119:LEU:HD11	1.99	0.43
1:B:94:LEU:HD11	1:B:164:VAL:HG22	2.00	0.43
1:D:100:ASN:N	1:D:101:PRO:HD3	2.33	0.43
1:D:164:VAL:O	1:D:168:LEU:HG	2.18	0.43
1:B:85:ARG:NH2	1:B:140:GLU:OE2	2.51	0.43
1:D:156:LEU:O	1:D:156:LEU:HD23	2.18	0.43
2:W:13:DT:C2	2:Z:27:DG:N2	2.85	0.43
1:C:163:GLN:HE21	1:D:159:GLN:HG3	1.79	0.43
1:D:21:LEU:O	1:D:105:ARG:HD2	2.19	0.43
1:D:86:ILE:HD11	1:D:138:LEU:HD23	2.00	0.43
1:D:123:ILE:HD13	1:D:123:ILE:HA	1.93	0.43
1:C:71:ARG:NH2	1:C:99:ARG:NH2	2.66	0.43
2:Z:23:DG:H2'	2:Z:24:DT:H72	1.99	0.43
1:A:42:SER:O	1:A:45:ALA:HB3	2.19	0.43
1:D:163:GLN:NE2	1:D:187:TYR:OH	2.50	0.43
1:C:156:LEU:O	1:C:160:LEU:HG	2.19	0.43
2:Z:27:DG:C2'	2:Z:28:DT:H5''	2.49	0.43
1:C:116:ASN:OD1	1:C:116:ASN:N	2.52	0.42
1:B:66:GLU:CB	3:B:225:HOH:O	2.67	0.42
1:C:196:LYS:O	1:C:196:LYS:HE2	2.19	0.42
1:D:154:ASN:N	1:D:154:ASN:HD22	2.17	0.42
1:B:123:ILE:HD13	1:B:123:ILE:HA	1.87	0.42
1:B:196:LYS:HE2	1:B:196:LYS:HB3	1.94	0.42
1:C:119:LEU:O	1:C:122:ARG:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:LEU:HD12	1:B:60:LEU:HA	1.82	0.42
2:Z:21:DA:H2''	2:Z:22:DC:O5'	2.19	0.42
1:A:17:LEU:O	1:A:21:LEU:HB2	2.20	0.42
1:C:53:LYS:O	1:C:56:MET:HB2	2.19	0.42
1:C:152:ASP:OD1	1:C:153:GLU:N	2.53	0.42
1:B:95:ALA:O	1:B:99:ARG:HG3	2.20	0.42
1:D:170:ARG:HG2	1:D:173:ARG:NH2	2.34	0.42
1:D:74:ARG:O	1:D:78:GLU:HG3	2.19	0.42
1:B:152:ASP:OD1	1:B:154:ASN:HB2	2.20	0.41
1:C:14:LEU:HD22	1:C:60:LEU:CD1	2.50	0.41
1:B:21:LEU:HD13	1:B:30:ILE:HD12	2.01	0.41
1:B:192:SER:O	1:B:196:LYS:HG3	2.21	0.41
1:D:55:ARG:HD3	1:D:55:ARG:HA	1.92	0.41
1:A:86:ILE:HG22	1:A:188:TRP:CZ3	2.55	0.41
1:D:79:GLU:O	1:D:85:ARG:HD2	2.19	0.41
1:D:97:ALA:CB	1:D:168:LEU:HD22	2.51	0.41
1:C:68:LEU:O	1:C:72:ILE:HG13	2.20	0.41
1:C:171:PHE:CD1	1:C:180:PRO:HD3	2.55	0.41
1:C:9:ARG:HG3	2:Z:23:DG:OP2	2.21	0.41
1:C:69:MET:HE3	1:C:126:LEU:HD11	2.02	0.41
1:C:163:GLN:OE1	1:C:163:GLN:HA	2.21	0.41
1:D:48:ARG:NH2	2:W:1:DT:H73	2.35	0.41
1:A:94:LEU:CD1	1:A:164:VAL:HG22	2.51	0.41
1:B:142:LYS:H	1:B:142:LYS:HG2	1.52	0.41
1:C:10:ARG:HG2	1:C:10:ARG:NH1	2.35	0.41
1:C:139:ARG:HH11	1:C:139:ARG:HG3	1.86	0.41
1:D:48:ARG:HH12	2:W:1:DT:H6	1.69	0.41
1:D:53:LYS:O	1:D:56:MET:HB2	2.20	0.41
2:Z:37:DA:H2''	2:Z:38:DA:OP2	2.21	0.41
1:A:186:GLU:N	1:A:186:GLU:OE1	2.54	0.41
1:B:22:GLU:HG3	1:B:101:PRO:HB2	2.02	0.40
1:C:14:LEU:HD22	1:C:60:LEU:HD13	2.03	0.40
1:C:99:ARG:C	1:C:101:PRO:HD3	2.46	0.40
1:A:43:GLU:HA	1:A:46:LEU:HD23	2.04	0.40
1:C:39:VAL:O	1:C:39:VAL:HG12	2.22	0.40
1:B:103:LEU:O	1:B:106:ILE:HB	2.21	0.40
1:C:73:ASN:HD22	1:C:73:ASN:HA	1.70	0.40
1:C:163:GLN:HE22	1:D:159:GLN:HG3	1.83	0.40
1:C:173:ARG:HB3	1:D:124:ASN:OD1	2.21	0.40
1:A:68:LEU:O	1:A:72:ILE:HG13	2.22	0.40

There are no symmetry-related clashes.

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	181/196 (92%)	174 (96%)	5 (3%)	2 (1%)	11	12
1	B	187/196 (95%)	177 (95%)	8 (4%)	2 (1%)	11	12
1	C	188/196 (96%)	178 (95%)	10 (5%)	0	100	100
1	D	187/196 (95%)	179 (96%)	8 (4%)	0	100	100
All	All	743/784 (95%)	708 (95%)	31 (4%)	4 (0%)	24	32

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	150	PRO
1	B	195	ILE
1	B	174	SER
1	A	149	PHE

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	160/171 (94%)	148 (92%)	12 (8%)	12	16
1	B	164/171 (96%)	144 (88%)	20 (12%)	5	4
1	C	167/171 (98%)	157 (94%)	10 (6%)	17	26
1	D	165/171 (96%)	145 (88%)	20 (12%)	5	4
All	All	656/684 (96%)	594 (90%)	62 (10%)	8	8

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLU
1	A	15	GLN
1	A	19	GLU
1	A	21	LEU
1	A	46	LEU
1	A	86	ILE
1	A	122	ARG
1	A	153	GLU
1	A	156	LEU
1	A	159	GLN
1	A	160	LEU
1	A	191	LEU
1	B	21	LEU
1	B	46	LEU
1	B	60	LEU
1	B	62	GLU
1	B	68	LEU
1	B	74	ARG
1	B	83	LEU
1	B	85	ARG
1	B	94	LEU
1	B	123	ILE
1	B	125	GLN
1	B	126	LEU
1	B	128	GLU
1	B	134	LEU
1	B	142	LYS
1	B	143	LEU
1	B	156	LEU
1	B	160	LEU
1	B	173	ARG
1	B	191	LEU
1	C	9	ARG
1	C	17	LEU
1	C	46	LEU
1	C	66	GLU
1	C	68	LEU
1	C	84	ASN
1	C	116	ASN
1	C	145	GLU
1	C	177	LYS
1	C	196	LYS

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Mol	Chain	Res	Type
1	D	21	LEU
1	D	43	GLU
1	D	60	LEU
1	D	84	ASN
1	D	85	ARG
1	D	86	ILE
1	D	92	LEU
1	D	115	GLU
1	D	117	GLU
1	D	125	GLN
1	D	126	LEU
1	D	134	LEU
1	D	136	GLN
1	D	141	ARG
1	D	147	LYS
1	D	152	ASP
1	D	154	ASN
1	D	160	LEU
1	D	191	LEU
1	D	196	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	24	ASN
1	A	73	ASN
1	A	125	GLN
1	A	136	GLN
1	A	159	GLN
1	A	163	GLN
1	A	183	ASN
1	B	124	ASN
1	B	154	ASN
1	B	159	GLN
1	B	169	ASN
1	B	194	GLN
1	C	15	GLN
1	C	49	HIS
1	C	73	ASN
1	C	91	GLN
1	C	159	GLN

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Mol	Chain	Res	Type
1	C	169	ASN
1	D	8	ASN
1	D	15	GLN
1	D	125	GLN
1	D	136	GLN
1	D	154	ASN
1	D	159	GLN
1	D	163	GLN
1	D	169	ASN
1	D	194	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	185/196 (94%)	0.14	8 (4%) 40 39	29, 42, 68, 111	0
1	B	189/196 (96%)	0.13	3 (1%) 70 73	27, 44, 67, 96	0
1	C	190/196 (96%)	0.21	6 (3%) 50 51	28, 45, 68, 88	0
1	D	189/196 (96%)	0.19	3 (1%) 70 73	23, 42, 67, 98	0
2	W	20/20 (100%)	0.39	1 (5%) 34 32	37, 57, 93, 102	0
2	Z	20/20 (100%)	0.32	1 (5%) 34 32	33, 58, 100, 115	0
All	All	793/824 (96%)	0.17	22 (2%) 55 56	23, 44, 71, 115	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	148	SER	4.8
1	A	147	LYS	4.3
1	C	7	ILE	4.0
1	D	25	GLU	3.6
1	A	7	ILE	3.6
1	A	149	PHE	3.5
1	B	117	GLU	3.4
2	Z	19	DT	2.9
1	A	54	THR	2.9
1	A	9	ARG	2.8
1	C	175	ASP	2.6
1	D	48	ARG	2.6
1	B	175	ASP	2.5
1	A	195	ILE	2.5
1	C	135	ARG	2.4
1	D	66	GLU	2.4
1	A	150	PRO	2.3
2	W	1	DT	2.2
1	C	136	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	54	THR	2.1
1	B	48	ARG	2.0
1	C	66	GLU	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.