W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

May 14, 2020 – 03:33 pm BST

PDB ID	:	5OXV
Title	:	Structure of the 4_601_157 tetranucleosome (C2 form)
Authors	:	Ekundayo, B.; Schalch, T.
Deposited on	:	2017-09-07
Resolution	:	6.72 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

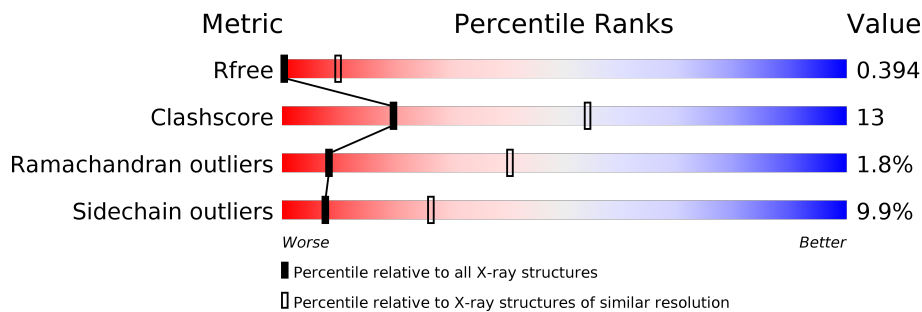|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 6.72 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	Percentile Ranks	Value
Rfree		0.394
Clashscore		13
Ramachandran outliers		1.8%
Sidechain outliers		9.9%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1002 (9.50-3.90)
Clashscore	141614	1066 (9.50-3.90)
Ramachandran outliers	138981	1000 (9.50-3.90)
Sidechain outliers	138945	1000 (9.50-3.86)

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 <=5%

Mol	Chain	Length	Quality of chain
1	J	312	44% 44% 12% •
2	D	126	43% 27% 5% • 25%
2	H	126	44% 27% • 26%
2	N	126	44% 26% 5% • 25%
2	R	126	44% 26% • 26%
3	C	130	51% 24% 5% 21%
3	G	130	48% 28% 5% 19%

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Mol	Chain	Length	Quality of chain
3	M	130	52% · · · 23% · 5% · 21%
3	Q	130	46% · · · 31% · · · 19%
4	B	102	44% · · · 32% · 5% · 19%
4	F	102	61% · · · 14% · · · 24%
4	L	102	44% · · · 32% · 5% · 19%
4	P	102	60% · · · 15% · · · 24%
5	A	135	49% · · · 19% · · · 28%
5	E	135	52% · · · 20% · · · 28%
5	K	135	49% · · · 19% · · · 28%
5	O	135	53% · · · 19% · · · 28%
6	I	313	45% · · · 42% · · · 12% ·

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 24648 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 DNA chain called DNA STRAND 1 (601-based sequence model).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	J	310	Total 6394	C 3024	N 1203	O 1857	P 310	0	0	0

- Molecule 2 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	R	93	Total 726	C 457	N 130	O 137	S 2	0	0	0
2	N	95	Total 745	C 469	N 134	O 140	S 2	0	0	0
2	H	93	Total 726	C 457	N 130	O 137	S 2	0	0	0
2	D	95	Total 745	C 469	N 134	O 140	S 2	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	29	THR	SER	conflict	UNP P02281
N	29	THR	SER	conflict	UNP P02281
H	29	THR	SER	conflict	UNP P02281
D	29	THR	SER	conflict	UNP P02281

- Molecule 3 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	Q	105	Total 809	C 510	N 158	O 141	0	0	0
3	M	103	Total 795	C 501	N 155	O 139	0	0	0
3	G	105	Total 809	C 510	N 158	O 141	0	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	103	Total 795	C 501	N 155	O 139	0	0	0

- Molecule 4 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	P	78	Total 619	C 391	N 120	O 107	S 1	0	0	0
4	L	83	Total 662	C 418	N 129	O 114	S 1	0	0	0
4	F	78	Total 619	C 391	N 120	O 107	S 1	0	0	0
4	B	83	Total 662	C 418	N 129	O 114	S 1	0	0	0

- Molecule 5 is a protein called Histone H3.2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	O	97	Total 801	C 504	N 155	O 139	S 3	0	0	0
5	K	97	Total 802	C 506	N 155	O 138	S 3	0	0	0
5	E	97	Total 801	C 504	N 155	O 139	S 3	0	0	0
5	A	97	Total 802	C 506	N 155	O 138	S 3	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	102	ALA	GLY	conflict	UNP P84233
K	102	ALA	GLY	conflict	UNP P84233
E	102	ALA	GLY	conflict	UNP P84233
A	102	ALA	GLY	conflict	UNP P84233

- Molecule 6 is a DNA chain called DNA STRAND 2 (601-based sequence model).

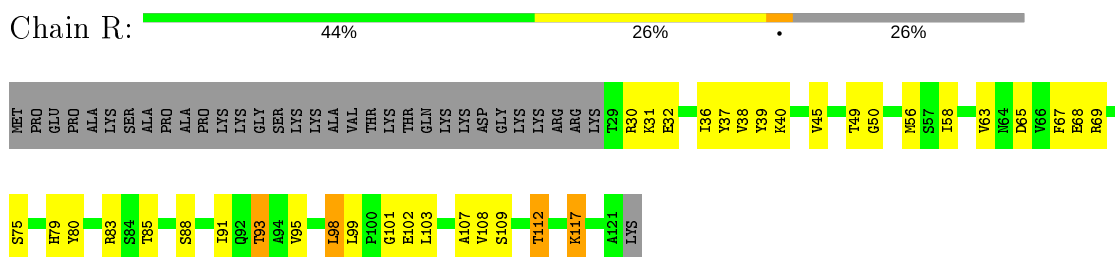| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	I	311	Total 6336	C 3009	N 1146	O 1870	P 311	0	0	0

3 Residue-property plots ⓘ

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. 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. 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.
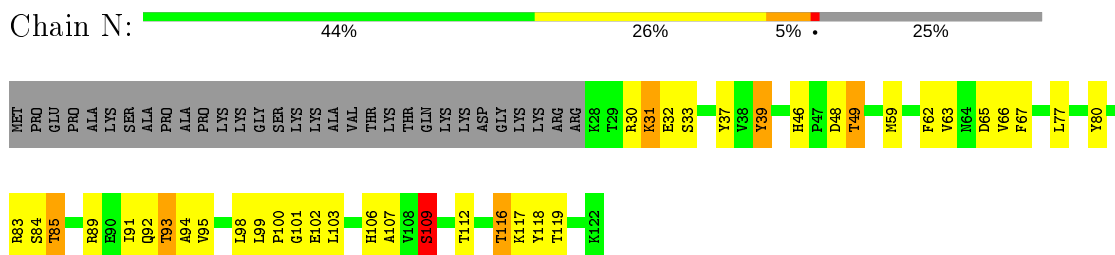
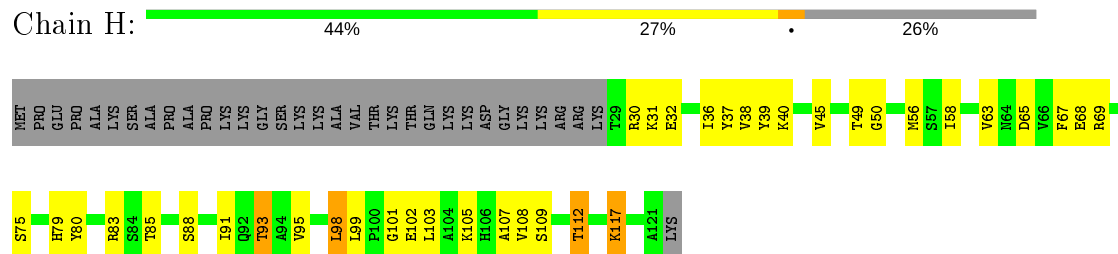- Molecule 1: DNA STRAND 1 (601-based sequence model)
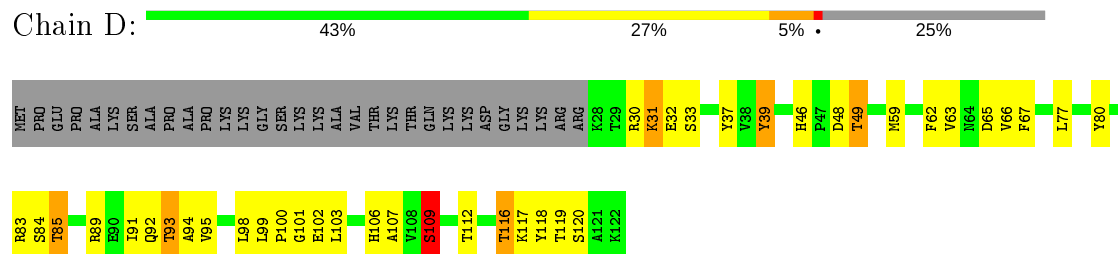
Chain J:

- Molecule 2: Histone H2B 1.1

Chain R:

- Molecule 2: Histone H2B 1.1

Chain N:

- Molecule 2: Histone H2B 1.1

Chain H:

44% 27% • 26%

MET PRO GLU PRO ALA LYS SER ALA PRO ALA PRO LYS LYS GLY SER LYS LYS ALA VAL THR LYS THR GLN LYS LYS ASP GLY LYS LYS ARG ARG LYS T29 R30 K31 E32 I36 Y37 V38 Y39 K40 V45 T49 G50 M56 S57 I58 V63 N64 D65 V66 F67 E68 R69

S75 H79 Y80 R83 S84 T85 S88 I91 Q92 T93 A94 V95 L98 L99 P100 G101 E102 L103 A104 K105 H106 A107 V108 S109 T112 K117 A121 LYS

• Molecule 2: Histone H2B 1.1

Chain D:

43% 27% 5% • 25%

MET PRO GLU PRO ALA LYS SER ALA PRO ALA PRO LYS LYS GLY SER LYS LYS ALA VAL THR LYS THR GLN LYS LYS ASP GLY LYS LYS ARG ARG K28 T29 R30 K31 E32 S33 Y37 V38 Y39 H46 P47 D48 T49 M59 F62 V63 N64 D65 V66 F67 L77 Y80

R83 S84 T85 R89 E90 I91 Q92 T93 A94 V95 L98 L99 P100 G101 E102 L103 H106 A107 V108 S109 T112 T116 K117 Y118 T119 S120 A121 K122

• Molecule 3: Histone H2A

Chain Q:

46% 31% • 19%

MET SER GLY ARG GLY LYS GLN GLY LYS LYS THR ARG ALA LYS A14 S19 G22 F25 P26 V30 H31 R32 L33 L34 R35 Y39 R42 V43 G44 A47 Y50 L51 V54 L55 E56 Y57 L58 T59 A60 E61 I62 L63 E64 L65 A66 A69 D72 N73 K74

K75 T76 R77 P80 R81 H82 L83 Q84 L85 A86 V87 R88 N89 D90 E91 E92 L93 L97 V100 T101 V107 V114 K118 LYS THR GLU SER SER LYS SER ALA LYS SER LYS

• Molecule 3: Histone H2A

Chain M:

52% 23% 5% 21%

MET SER GLY ARG GLY LYS GLN GLY LYS LYS THR ARG ALA LYS ALA LYS T16 R17 S18 S19 R20 F25 P26 V27 G28 R29 R32 R35 N38 R42 A47 P48 V49 Y50 V54 L55 T59 E64 I79 P80 R81 H82 L83 V87 E91 E92 L93 N94

K95 L96 L97 G98 T101 S113 V114 L115 K118 LYS THR GLU SER SER LYS SER ALA LYS SER LYS

• Molecule 3: Histone H2A

Chain G:

48% 28% 5% 19%

MET SER GLY ARG GLY LYS GLN GLY LYS LYS THR ARG ALA LYS A14 S19 F25 P26 V30 H31 R32 L33 L34 R35 Y39 R42 V43 G44 A47 Y50 L51 V54 L55 E56 Y57 L58 T59 A60 E61 I62 L63 E64 D72 N73 K74 K75 T76 R77 P80 R81

H82 L83 Q84 L85 A86 V87 R88 N89 D90 E91 E92 L93 L97 V100 T101 V107 V114 K118 LYS THR GLU SER SER LYS SER ALA LYS SER LYS

• Molecule 3: Histone H2A

Chain C:

51% 24% 5% 21%

MET SER GLY ARG GLY LYS GLN GLY GLY LYS THR ARG ALA LYS ALA LYS **T16** **R17** R20 **F25** **P26** **V27** **G28** **R29** R32 R35 N38 R42 A47 P48 V49 Y50 V54 L55 **T59** E64 A69 N73 I79 P80 R81 **H82** L83 V87 E91

E92 L93 **N94** K95 L96 L97 G98 T101 **S113** **V114** L115 **K118** LYS THR GLU SER SER LYS SER ALA LYS SER LYS

● Molecule 4: Histone H4

Chain P:

60% 15% • 24%

SER GLY ARG GLY LYS GLY LYS GLY LEU GLY LYS GLY GLY ALA LYS ARG HIS ARG LYS VAL LEU ARG ASP **N25** **I26** R35 R40 E53 T54 R55 G56 V57 L58 K59 E63 T73 E74 H75 K79 A83 Y88 A89 **R92** Y98 G102

● Molecule 4: Histone H4

Chain L:

44% 32% 5% 19%

SER GLY ARG GLY LYS GLY LYS GLY LEU GLY LYS GLY GLY ALA LYS ARG HIS ARG **K20** **I26** **Q27** **G28** **I29** T30 K31 P32 A33 **I34** R35 R36 R39 R40 G41 R45 **I46** **S47** Y51 R55 I66 R67 D68 A69 V70 T73 E74 H75 A76 K77 R78 K79 T80 V81

T82 D85 Y88 A89 L90 K91 **R92** R95 T96 L97 Y98 G99 F100 G101 G102
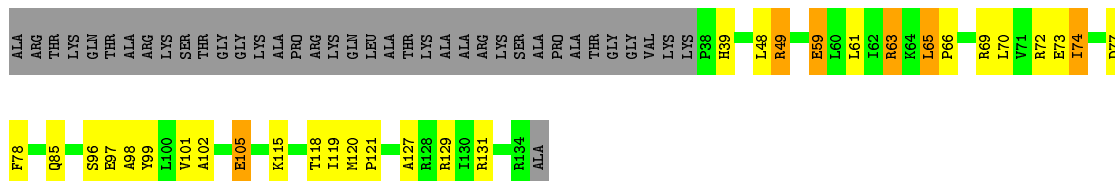
● Molecule 4: Histone H4

Chain F:

61% 14% • 24%

SER GLY ARG GLY LYS GLY LYS GLY LEU GLY LYS GLY GLY ALA LYS ARG HIS ARG LYS VAL LEU ARG ASP **N25** **I26** R35 E53 T54 R55 G56 V57 L58 K59 E63 T73 E74 H75 K79 A83 Y88 A89 **R92** Y98 G102

● Molecule 4: Histone H4

Chain B:

44% 32% 5% 19%

SER GLY ARG GLY LYS GLY LYS GLY LEU GLY LYS GLY GLY ALA LYS ARG HIS ARG **K20** **I26** **Q27** **G28** **I29** T30 K31 P32 A33 **I34** R35 R36 R39 R40 G41 R45 **I46** **S47** Y51 R55 I66 R67 D68 A69 V70 T73 E74 H75 A76 K77 R78 K79 T80 V81

T82 D85 Y88 A89 L90 K91 **R92** R95 T96 L97 Y98 G99 F100 G101 G102

● Molecule 5: Histone H3.2

Chain O:

53% 19% • 28%

ALA ARG THR LYS GLN THR ALA ARG LYS SER THR GLY GLY LYS ALA PRO ARG LYS GLN LEU ALA THR LYS ALA ALA ARG LYS SER ALA PRO ALA THR GLY GLY VAL LYS LYS PRO **H39** R42 P43 L48 I51 R52 Q55 **E59** L60 I65 **P66** F67 V71 K79

L82 S87 Q93 V101 A102 E105 C110 V117 P121 L126 A127 R128 R129 R134 A135

- Molecule 5: Histone H3.2

Chain K:

49% 19% 28%

- Molecule 5: Histone H3.2

Chain E:

52% 20% 28%

- Molecule 5: Histone H3.2

Chain A:

49% 19% 28%
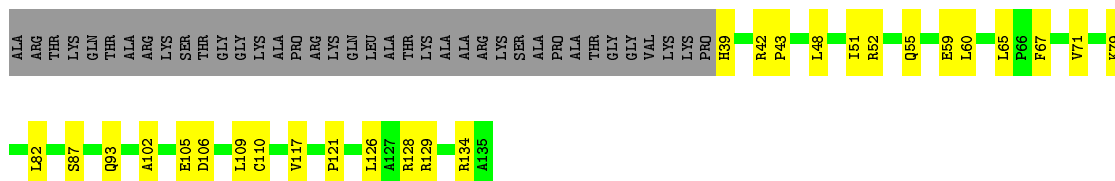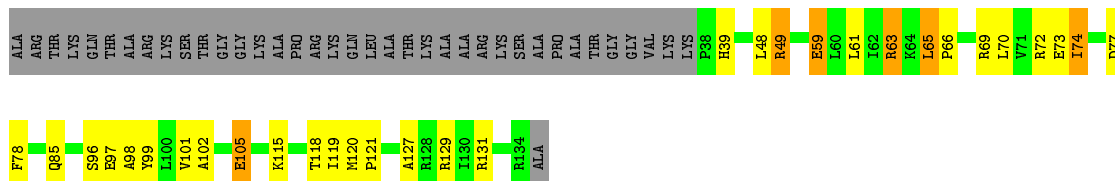
- Molecule 6: DNA STRAND 2 (601-based sequence model)

Chain I:

45% 42% 12%
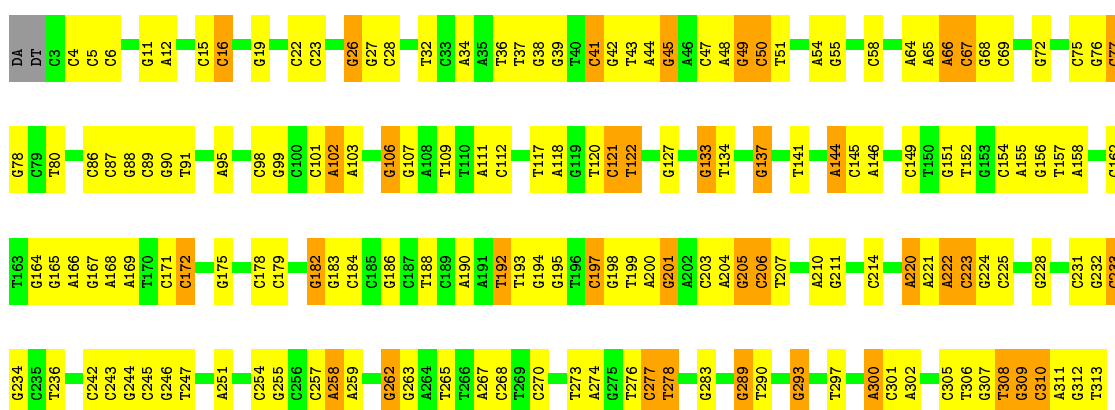
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	348.84Å 63.27Å 271.36Å 90.00° 124.74° 90.00°	Depositor
Resolution (Å)	71.67 – 6.72 222.99 – 6.72	Depositor EDS
% Data completeness (in resolution range)	87.8 (71.67-6.72) 82.3 (222.99-6.72)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	0.22 (at 6.74Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.317 , 0.352 0.358 , 0.394	Depositor DCC
R_{free} test set	1169 reflections (12.72%)	wwPDB-VP
Wilson B-factor (Å^2)	308.9	Xtriage
Anisotropy	0.465	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	1.04 , -10.0	EDS
L-test for twinning[2]	$<|L|> = 0.45, <L^2> = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.79	EDS
Total number of atoms	24648	wwPDB-VP
Average B, all atoms (Å^2)	637.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.99% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $<|L|>$, $<L^2>$ 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	J	0.74	2/7182 (0.0%)	1.47	96/11093 (0.9%)
2	D	0.49	0/756	0.64	0/1015
2	H	0.62	0/737	0.70	0/993
2	N	0.49	0/756	0.64	0/1015
2	R	0.62	0/737	0.70	0/993
3	C	0.42	0/805	0.61	0/1088
3	G	0.62	0/819	0.76	0/1106
3	M	0.43	0/805	0.61	0/1088
3	Q	0.63	0/819	0.76	0/1106
4	B	0.67	0/669	0.84	0/894
4	F	0.46	0/626	0.61	0/837
4	L	0.67	0/669	0.84	0/894
4	P	0.45	0/626	0.61	0/837
5	A	0.66	0/814	0.73	0/1092
5	E	0.41	0/812	0.58	0/1088
5	K	0.66	0/814	0.73	0/1092
5	O	0.41	0/812	0.58	0/1088
6	I	0.74	4/7098 (0.1%)	1.38	84/10943 (0.8%)
All	All	0.66	6/26356 (0.0%)	1.17	180/38262 (0.5%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	-310	DG	C1'-N9	-6.27	1.38	1.47
6	I	310	DC	C1'-N1	5.73	1.56	1.49
1	J	-305	DG	C1'-N9	-5.53	1.39	1.47
6	I	312	DG	C1'-N9	-5.43	1.39	1.47
6	I	308	DT	C1'-N1	5.30	1.56	1.49

The worst 5 of 180 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	-163	DA	O3'-P-O5'	33.99	168.59	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	-163	DA	P-O3'-C3'	29.81	155.47	119.70
1	J	-163	DA	OP1-P-O3'	-20.17	60.83	105.20
6	I	162	DC	O3'-P-O5'	14.02	130.63	104.00
1	J	-163	DA	OP2-P-O3'	-12.28	78.18	105.20

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	J	6394	0	3474	141	2
2	D	745	0	773	37	3
2	H	726	0	747	36	2
2	N	745	0	773	36	2
2	R	726	0	747	35	2
3	C	795	0	846	25	0
3	G	809	0	864	43	1
3	M	795	0	846	26	1
3	Q	809	0	864	44	1
4	B	662	0	709	36	0
4	F	619	0	659	16	0
4	L	662	0	709	36	0
4	P	619	0	659	17	0
5	A	802	0	841	22	0
5	E	801	0	838	15	0
5	K	802	0	841	21	0
5	O	801	0	838	17	0
6	I	6336	0	3489	146	2
All	All	24648	0	19517	554	8

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 13.

The worst 5 of 554 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)
2:D:93:THR:HG21	4:B:75:HIS:CD2	1.58	1.37
2:N:93:THR:HG21	4:L:75:HIS:CD2	1.58	1.37
1:J:-306:DA:C2	6:I:307:DG:N2	1.97	1.32
1:J:-306:DA:H2	6:I:307:DG:C2	1.48	1.29
1:J:-306:DA:C2	6:I:307:DG:C2	2.28	1.21

The worst 5 of 8 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)
2:H:117:LYS:CE	2:D:117:LYS:NZ[1_545]	1.23	0.97
1:J:-312:DC:P	6:I:313:DT:O3'[2_656]	1.61	0.59
1:J:-312:DC:OP2	6:I:313:DT:O3'[2_656]	1.79	0.41
2:H:117:LYS:CE	2:D:117:LYS:CE[1_545]	1.86	0.34
2:R:117:LYS:CE	2:N:117:LYS:NZ[1_565]	1.90	0.30

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	
2	D	93/126 (74%)	82 (88%)	9 (10%)	2 (2%)	6	35
2	H	91/126 (72%)	79 (87%)	11 (12%)	1 (1%)	14	52
2	N	93/126 (74%)	81 (87%)	10 (11%)	2 (2%)	6	35
2	R	91/126 (72%)	80 (88%)	10 (11%)	1 (1%)	14	52
3	C	101/130 (78%)	88 (87%)	9 (9%)	4 (4%)	3	23
3	G	103/130 (79%)	88 (85%)	15 (15%)	0	100	100
3	M	101/130 (78%)	88 (87%)	9 (9%)	4 (4%)	3	23
3	Q	103/130 (79%)	88 (85%)	15 (15%)	0	100	100
4	B	81/102 (79%)	70 (86%)	8 (10%)	3 (4%)	3	24
4	F	76/102 (74%)	67 (88%)	9 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	L	81/102 (79%)	70 (86%)	8 (10%)	3 (4%)	3	24
4	P	76/102 (74%)	67 (88%)	9 (12%)	0	100	100
5	A	95/135 (70%)	83 (87%)	9 (10%)	3 (3%)	4	26
5	E	95/135 (70%)	86 (90%)	9 (10%)	0	100	100
5	K	95/135 (70%)	83 (87%)	9 (10%)	3 (3%)	4	26
5	O	95/135 (70%)	86 (90%)	9 (10%)	0	100	100
All	All	1470/1972 (74%)	1286 (88%)	158 (11%)	26 (2%)	8	40

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	N	101	GLY
4	L	29	ILE
5	K	73	GLU
2	D	101	GLY
4	B	29	ILE

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	
2	D	81/106 (76%)	69 (85%)	12 (15%)	3	15
2	H	79/106 (74%)	67 (85%)	12 (15%)	3	14
2	N	81/106 (76%)	69 (85%)	12 (15%)	3	15
2	R	79/106 (74%)	67 (85%)	12 (15%)	3	14
3	C	82/102 (80%)	75 (92%)	7 (8%)	10	33
3	G	83/102 (81%)	74 (89%)	9 (11%)	6	23
3	M	82/102 (80%)	75 (92%)	7 (8%)	10	33
3	Q	83/102 (81%)	74 (89%)	9 (11%)	6	23
4	B	68/78 (87%)	63 (93%)	5 (7%)	13	38
4	F	63/78 (81%)	59 (94%)	4 (6%)	18	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	L	68/78 (87%)	63 (93%)	5 (7%)	13	38
4	P	63/78 (81%)	59 (94%)	4 (6%)	18	43
5	A	85/110 (77%)	77 (91%)	8 (9%)	8	28
5	E	84/110 (76%)	79 (94%)	5 (6%)	19	44
5	K	85/110 (77%)	77 (91%)	8 (9%)	8	28
5	O	84/110 (76%)	79 (94%)	5 (6%)	19	44
All	All	1250/1584 (79%)	1126 (90%)	124 (10%)	8	26

5 of 124 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	K	59	GLU
2	H	98	LEU
4	B	91	LYS
5	K	63	ARG
2	H	31	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
3	G	31	HIS
3	G	84	GLN
3	C	112	GLN
4	L	75	HIS
3	C	73	ASN

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 (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.