wwPDB X-ray Structure Validation Summary Report (i)

Nov 20, 2023 – 01:09 PM EST

PDB ID	:	3VD2
Title	:	structure of p73 DNA binding domain tetramer modulates p73 transactivation
Authors	:	Ethayathulla, A.S.; Tse, P.W.; Nguyen, S.; Viadiu, H.
Deposited on	:	2012-01-04
Resolution	:	4.00 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

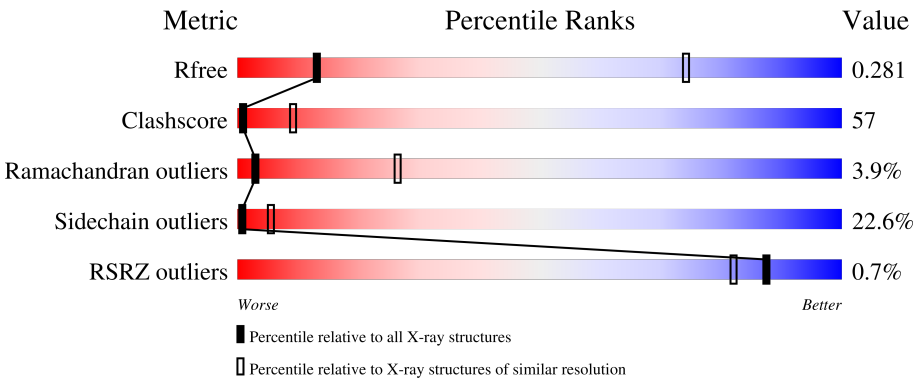
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 4.00 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	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)

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 <=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	210	29% 51% 15% • •
1	B	210	21% 56% 18% • 5%
1	C	210	32% 50% 13% •
1	D	210	% 31% 50% 14% 5%
1	I	210	% 20% 56% 19% • •

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Mol	Chain	Length	Quality of chain
1	J	210	29% 47% 20%
2	E	14	14% 29% 71%
2	F	14	14% 79% 7%
2	G	14	7% 86% 7%
2	H	14	21% 79%
2	K	14	7% 64% 21% 7%
2	L	14	7% 21% 50% 21% 7%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 11152 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 Tumor protein p73.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	203	1590	994	289	296	11	0	0	0
1	B	200	1569	981	283	294	11	0	0	0
1	C	203	1596	997	291	297	11	0	0	0
1	D	199	1563	981	282	289	11	0	0	0
1	I	202	1576	985	284	296	11	0	0	0
1	J	202	1586	993	284	298	11	0	0	0

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	103	MET	-	initiating methionine	UNP O15350
A	104	GLY	-	expression tag	UNP O15350
A	105	HIS	-	expression tag	UNP O15350
A	106	HIS	-	expression tag	UNP O15350
A	107	HIS	-	expression tag	UNP O15350
A	108	HIS	-	expression tag	UNP O15350
A	109	HIS	-	expression tag	UNP O15350
A	110	HIS	-	expression tag	UNP O15350
A	111	HIS	-	expression tag	UNP O15350
A	112	HIS	-	expression tag	UNP O15350
A	113	GLU	-	expression tag	UNP O15350
A	114	PHE	-	expression tag	UNP O15350
B	103	MET	-	initiating methionine	UNP O15350
B	104	GLY	-	expression tag	UNP O15350
B	105	HIS	-	expression tag	UNP O15350
B	106	HIS	-	expression tag	UNP O15350
B	107	HIS	-	expression tag	UNP O15350

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Chain	Residue	Modelled	Actual	Comment	Reference
B	108	HIS	-	expression tag	UNP O15350
B	109	HIS	-	expression tag	UNP O15350
B	110	HIS	-	expression tag	UNP O15350
B	111	HIS	-	expression tag	UNP O15350
B	112	HIS	-	expression tag	UNP O15350
B	113	GLU	-	expression tag	UNP O15350
B	114	PHE	-	expression tag	UNP O15350
C	103	MET	-	initiating methionine	UNP O15350
C	104	GLY	-	expression tag	UNP O15350
C	105	HIS	-	expression tag	UNP O15350
C	106	HIS	-	expression tag	UNP O15350
C	107	HIS	-	expression tag	UNP O15350
C	108	HIS	-	expression tag	UNP O15350
C	109	HIS	-	expression tag	UNP O15350
C	110	HIS	-	expression tag	UNP O15350
C	111	HIS	-	expression tag	UNP O15350
C	112	HIS	-	expression tag	UNP O15350
C	113	GLU	-	expression tag	UNP O15350
C	114	PHE	-	expression tag	UNP O15350
D	103	MET	-	initiating methionine	UNP O15350
D	104	GLY	-	expression tag	UNP O15350
D	105	HIS	-	expression tag	UNP O15350
D	106	HIS	-	expression tag	UNP O15350
D	107	HIS	-	expression tag	UNP O15350
D	108	HIS	-	expression tag	UNP O15350
D	109	HIS	-	expression tag	UNP O15350
D	110	HIS	-	expression tag	UNP O15350
D	111	HIS	-	expression tag	UNP O15350
D	112	HIS	-	expression tag	UNP O15350
D	113	GLU	-	expression tag	UNP O15350
D	114	PHE	-	expression tag	UNP O15350
I	103	MET	-	initiating methionine	UNP O15350
I	104	GLY	-	expression tag	UNP O15350
I	105	HIS	-	expression tag	UNP O15350
I	106	HIS	-	expression tag	UNP O15350
I	107	HIS	-	expression tag	UNP O15350
I	108	HIS	-	expression tag	UNP O15350
I	109	HIS	-	expression tag	UNP O15350
I	110	HIS	-	expression tag	UNP O15350
I	111	HIS	-	expression tag	UNP O15350
I	112	HIS	-	expression tag	UNP O15350
I	113	GLU	-	expression tag	UNP O15350

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Chain	Residue	Modelled	Actual	Comment	Reference
I	114	PHE	-	expression tag	UNP O15350
J	103	MET	-	initiating methionine	UNP O15350
J	104	GLY	-	expression tag	UNP O15350
J	105	HIS	-	expression tag	UNP O15350
J	106	HIS	-	expression tag	UNP O15350
J	107	HIS	-	expression tag	UNP O15350
J	108	HIS	-	expression tag	UNP O15350
J	109	HIS	-	expression tag	UNP O15350
J	110	HIS	-	expression tag	UNP O15350
J	111	HIS	-	expression tag	UNP O15350
J	112	HIS	-	expression tag	UNP O15350
J	113	GLU	-	expression tag	UNP O15350
J	114	PHE	-	expression tag	UNP O15350

- Molecule 2 is a DNA chain called DNA (5'-D(*AP*TP*GP*GP*AP*CP*AP*TP*GP*TP*CP*CP*AP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	E	14	284	137	52	82	13	0	0	0
2	F	14	284	137	52	82	13	0	0	0
2	G	14	284	137	52	82	13	0	0	0
2	H	14	284	137	52	82	13	0	0	0
2	L	13	266	127	47	79	13	0	0	0
2	K	13	264	127	50	75	12	0	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	A	1	1	1	0	0
3	B	1	1	1	0	0
3	C	1	1	1	0	0
3	D	1	1	1	0	0

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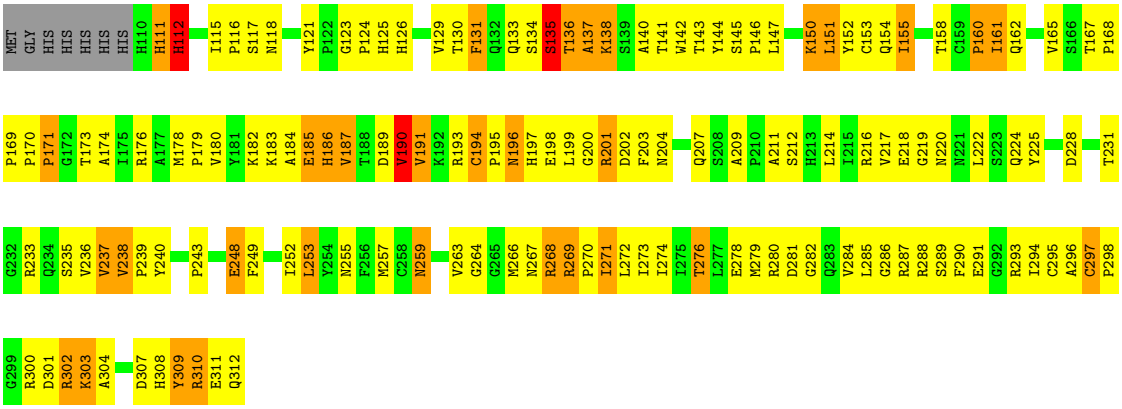
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	I	1	1	1	0	0
			Total	Zn		
3	J	1	1	1	0	0

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.

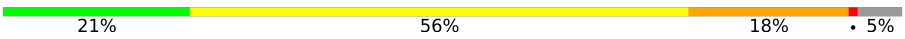
- Molecule 1: Tumor protein p73

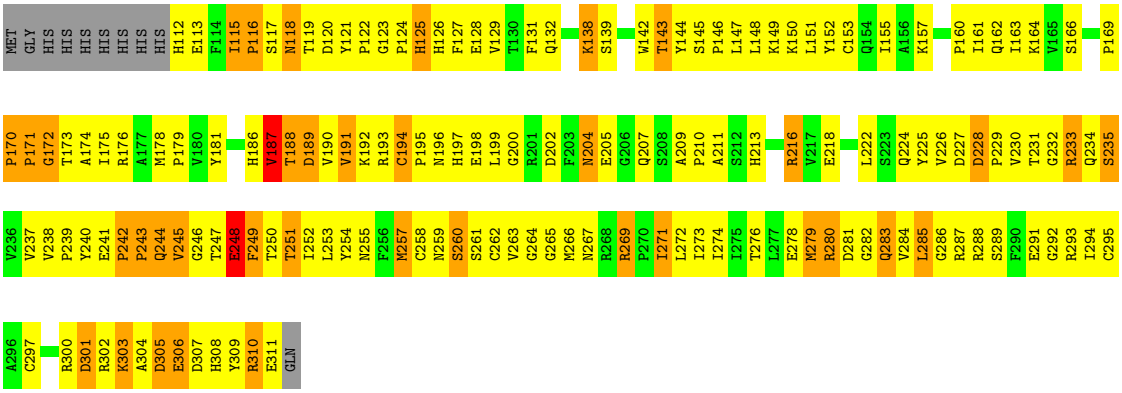
Chain A:



- Molecule 1: Tumor protein p73

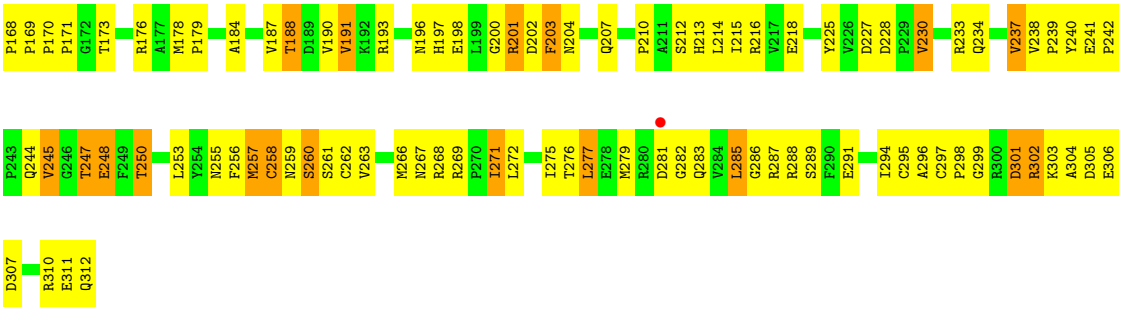
Chain B:





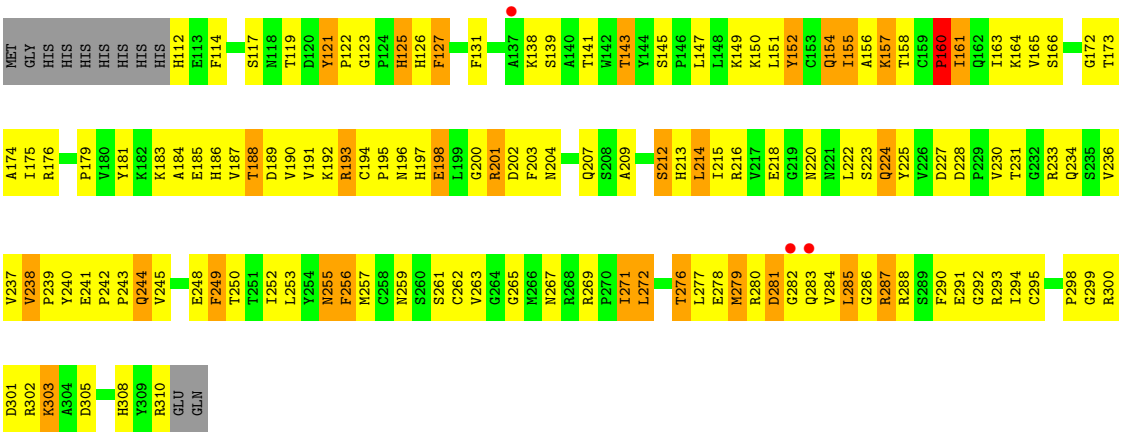
- Molecule 1: Tumor protein p73

Chain C:



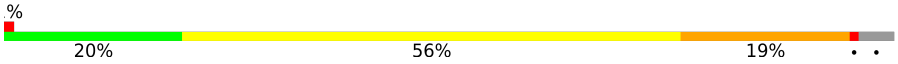
• Molecule 1: Tumor protein p73

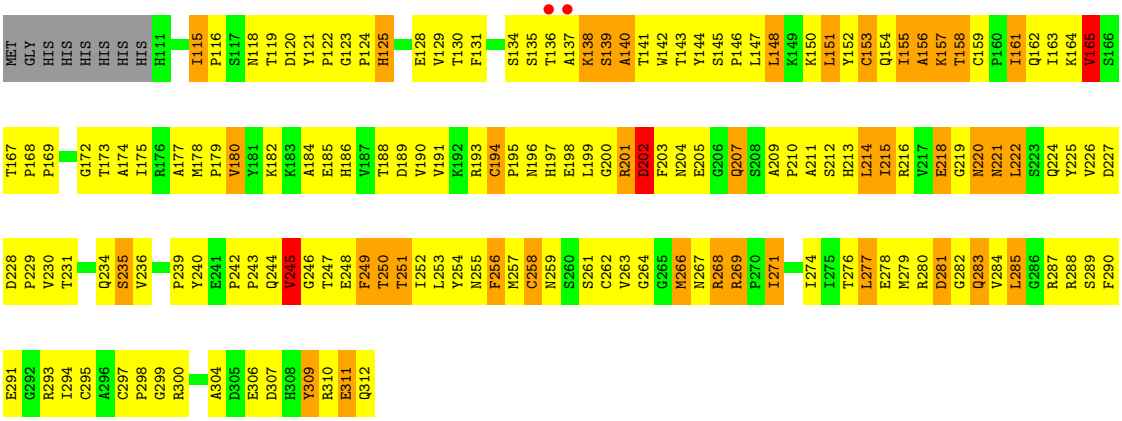
Chain D:



• Molecule 1: Tumor protein p73

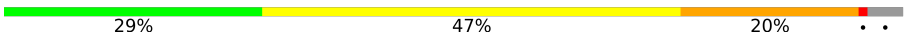
Chain I:





• Molecule 1: Tumor protein p73

Chain J:



V165 S166 T167 P168 P169 P170 T173 A174 I175 M178 P179 V180 Y181 K182 K183 A184 E185 H186 V187 T188 D189 V190 V191 K192 R193 C194 P195 N196 H197 E198 L199 G200 R201 D202 F203 N204 E205 G206 P210 A211 S212 H213 L214 I215 R216 V217 N220 N221 L222 Y225 V226 D227 T231 G232

R233 Q234 S235 V236 V237 V238 P239 Y240 E241 P242 P243 Q244 V245 T250 L253 Y254 N255 F256 M257 C258 N259 S260 S261 C262 V263 G264 G265 M266 N267 R268 R269 P270 I271 L272 I273 I274 I275 T276 L277 E278 M279 R280 D281 G282 L285 G286 R287 R288 E291 G292 R293 I294 C295 A296 C297 P298

G299 R300 D301 R302 K303 E311 Q312

- Molecule 2: DNA (5'-D(*AP*TP*GP*GP*AP*CP*AP*TP*GP*TP*CP*CP*AP*T)-3')

Chain E: 14% 29% 71%

A402 T403 G404 G405 A406 C407 A408 T409 G410 T411 T415

- Molecule 2: DNA (5'-D(*AP*TP*GP*GP*AP*CP*AP*TP*GP*TP*CP*CP*AP*T)-3')

Chain F: 14% 79% 7%

A500 T501 G502 G503 A504 C505 A506 T507 G508 C511 A512 T513

- Molecule 2: DNA (5'-D(*AP*TP*GP*GP*AP*CP*AP*TP*GP*TP*CP*CP*AP*T)-3')

Chain G: 7% 86% 7%

A602 T603 G604 G605 A606 C607 A608 T609 G610 T611 C612 C613 A614 T615

- Molecule 2: DNA (5'-D(*AP*TP*GP*GP*AP*CP*AP*TP*GP*TP*CP*CP*AP*T)-3')

Chain H: 21% 79%

A700 T701 G702 G703 A704 C705 A706 T707 G708 C711 A712 T713

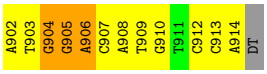
- Molecule 2: DNA (5'-D(*AP*TP*GP*GP*AP*CP*AP*TP*GP*TP*CP*CP*AP*T)-3')

Chain L: 7% 21% 50% 21% 7%

DA T801 G802 G803 A806 T807 G808 T809 C810 C811 A812 T813

- Molecule 2: DNA (5'-D(*AP*TP*GP*GP*AP*CP*AP*TP*GP*TP*CP*CP*AP*T)-3')

Chain K: 7% 64% 21% 7%


A902
T903
G904
G905
A906
C907
A908
T909
G910
T911
C912
C913
A914
DT

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	158.40Å 91.13Å 137.47Å 90.00° 90.20° 90.00°	Depositor
Resolution (Å)	45.69 – 4.00 45.69 – 4.00	Depositor EDS
% Data completeness (in resolution range)	99.1 (45.69-4.00) 98.1 (45.69-4.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	3.59 (at 4.00Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.248 , 0.284 0.246 , 0.281	Depositor DCC
R_{free} test set	350 reflections (2.10%)	wwPDB-VP
Wilson B-factor (Å^2)	91.2	Xtriage
Anisotropy	0.255	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.21 , -0.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.019 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.018 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.429 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.429 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.020 for -h,-k,l	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	11152	wwPDB-VP
Average B, all atoms (Å^2)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.15% of the height of the origin peak. No significant pseudotranslation is detected.*

[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)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.53	0/1631	0.87	3/2218 (0.1%)
1	B	0.46	0/1609	0.93	2/2187 (0.1%)
1	C	0.49	0/1638	0.83	2/2226 (0.1%)
1	D	0.49	0/1604	0.81	0/2181
1	I	0.51	0/1615	0.86	5/2195 (0.2%)
1	J	0.49	0/1626	0.83	2/2209 (0.1%)
2	E	0.59	0/318	0.92	0/489
2	F	0.71	0/318	0.98	1/489 (0.2%)
2	G	0.71	0/318	1.01	2/489 (0.4%)
2	H	0.63	0/318	0.96	0/489
2	K	1.03	1/296 (0.3%)	1.29	2/455 (0.4%)
2	L	1.10	0/297	1.40	7/456 (1.5%)
All	All	0.56	1/11588 (0.0%)	0.91	26/16083 (0.2%)

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	F	0	1
2	K	0	1
2	L	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	905	DG	C2'-C1'	-5.78	1.46	1.52

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	242	PRO	C-N-CD	-12.21	93.73	120.60
1	J	115	ILE	C-N-CD	-10.49	97.52	120.60
2	L	810	DC	O5'-P-OP2	8.05	120.36	110.70
2	L	810	DC	OP2-P-O3'	7.14	120.90	105.20
2	G	602	DA	O3'-P-O5'	-6.97	90.77	104.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	506	DA	Sidechain
2	K	904	DG	Sidechain
2	L	809	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	1590	0	1549	192	0
1	B	1569	0	1535	233	0
1	C	1596	0	1554	152	0
1	D	1563	0	1533	194	0
1	I	1576	0	1537	202	0
1	J	1586	0	1548	175	0
2	E	284	0	160	12	0
2	F	284	0	160	18	0
2	G	284	0	160	19	0
2	H	284	0	160	16	0
2	K	264	0	148	14	0
2	L	266	0	148	16	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
All	All	11152	0	10192	1211	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 57.

The worst 5 of 1211 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:176:ARG:HG3	1:B:237:VAL:HG22	1.32	1.10
1:B:163:ILE:O	1:B:249:PHE:HB2	1.56	1.06
1:I:243:PRO:HB2	1:I:246:GLY:HA2	1.36	1.04
1:I:215:ILE:HD13	1:I:215:ILE:H	1.17	1.03
1:J:214:LEU:HD23	1:J:215:ILE:HG13	1.39	1.03

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	201/210 (96%)	162 (81%)	31 (15%)	8 (4%)	3 26
1	B	198/210 (94%)	150 (76%)	35 (18%)	13 (7%)	1 17
1	C	201/210 (96%)	158 (79%)	40 (20%)	3 (2%)	10 45
1	D	197/210 (94%)	152 (77%)	38 (19%)	7 (4%)	3 28
1	I	200/210 (95%)	159 (80%)	33 (16%)	8 (4%)	3 26
1	J	200/210 (95%)	161 (80%)	31 (16%)	8 (4%)	3 26
All	All	1197/1260 (95%)	942 (79%)	208 (17%)	47 (4%)	3 26

5 of 47 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	136	THR
1	B	170	PRO
1	B	243	PRO

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Mol	Chain	Res	Type
1	B	245	VAL
1	B	248	GLU

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	177/186 (95%)	140 (79%)	37 (21%)	1 6
1	B	176/186 (95%)	137 (78%)	39 (22%)	1 6
1	C	178/186 (96%)	145 (82%)	33 (18%)	1 10
1	D	175/186 (94%)	139 (79%)	36 (21%)	1 7
1	I	175/186 (94%)	128 (73%)	47 (27%)	0 3
1	J	177/186 (95%)	130 (73%)	47 (27%)	0 3
All	All	1058/1116 (95%)	819 (77%)	239 (23%)	1 5

5 of 239 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	152	TYR
1	J	241	GLU
1	D	305	ASP
1	J	237	VAL
1	J	300	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	154	GLN
1	J	186	HIS
1	J	259	ASN
1	C	111	HIS
1	B	283	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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)

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	203/210 (96%)	-0.38	0	100	100	45, 74, 104, 125	3 (1%)
1	B	200/210 (95%)	-0.33	0	100	100	67, 88, 112, 123	1 (0%)
1	C	203/210 (96%)	-0.33	1 (0%)	91	85	50, 77, 103, 123	2 (0%)
1	D	199/210 (94%)	-0.20	3 (1%)	73	64	60, 87, 118, 127	2 (1%)
1	I	202/210 (96%)	-0.33	2 (0%)	82	74	57, 84, 111, 125	2 (0%)
1	J	202/210 (96%)	-0.35	0	100	100	54, 78, 108, 132	2 (0%)
2	E	14/14 (100%)	0.41	2 (14%)	2	3	76, 98, 132, 142	0
2	F	14/14 (100%)	-0.25	0	100	100	76, 104, 126, 137	0
2	G	14/14 (100%)	-0.31	0	100	100	74, 102, 142, 159	0
2	H	14/14 (100%)	-0.15	0	100	100	76, 100, 140, 151	0
2	K	13/14 (92%)	0.20	0	100	100	81, 103, 122, 137	0
2	L	13/14 (92%)	0.20	1 (7%)	13	11	90, 109, 135, 148	0
All	All	1291/1344 (96%)	-0.30	9 (0%)	87	82	45, 83, 117, 159	12 (0%)

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	136	THR	4.6
1	C	281	ASP	3.2
1	I	137	ALA	2.9
1	D	283	GLN	2.9
2	E	410	DG	2.6

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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ZN	D	401	1/1	0.97	0.05	84,84,84,84	0
3	ZN	B	401	1/1	0.98	0.14	89,89,89,89	0
3	ZN	C	401	1/1	0.98	0.09	58,58,58,58	0
3	ZN	A	401	1/1	0.98	0.08	73,73,73,73	0
3	ZN	I	401	1/1	0.98	0.07	76,76,76,76	0
3	ZN	J	401	1/1	1.00	0.15	56,56,56,56	0

6.5 Other polymers (i)

There are no such residues in this entry.