



wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 05:58 am BST

PDB ID : 4POG
Title : MCM-ssDNA co-crystal structure
Authors : Froelich, C.A.; Kang, S.; Epling, L.B.; Bell, S.P.; Enemark, E.J.
Deposited on : 2014-02-25
Resolution : 3.20 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 ⓘ symbol.

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

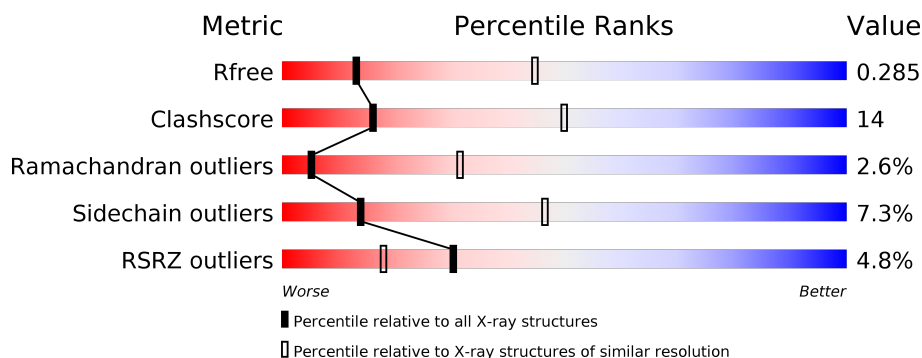
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 $\leq 5\%$. 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	257	<div> <div>6%</div> <div> <div></div> <div>70%</div> <div>26%</div> <div>...</div> </div> </div>
1	B	257	<div> <div>3%</div> <div> <div></div> <div>65%</div> <div>28%</div> <div>5%</div> <div>.</div> </div> </div>
1	C	257	<div> <div>4%</div> <div> <div></div> <div>69%</div> <div>25%</div> <div>5%</div> <div>.</div> </div> </div>
1	D	257	<div> <div>4%</div> <div> <div></div> <div>65%</div> <div>30%</div> <div>5%</div> <div>.</div> </div> </div>
1	E	257	<div> <div>5%</div> <div> <div></div> <div>67%</div> <div>30%</div> <div>..</div> </div> </div>
1	F	257	<div> <div>2%</div> <div> <div></div> <div>68%</div> <div>28%</div> <div>..</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	257	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>5%56%34%7%.</div></div>
1	H	257	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>9%65%29%5%.</div></div>
1	I	257	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>7%67%28%. .</div></div>
1	J	257	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>5%67%28%. .</div></div>
1	K	257	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>2%63%31%5%.</div></div>
1	L	257	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>4%63%31%5%.</div></div>
2	V	30	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>10%.87%</div></div>
2	X	30	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>.17%.77%</div></div>
2	Y	30	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>.23%10%63%</div></div>
2	Z	30	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>3%10%13%77%</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24942 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 Cell division control protein 21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	0	0	0
			2042	1294	350	389	9			
1	B	255	Total	C	N	O	S	0	0	0
			2042	1294	350	389	9			
1	C	255	Total	C	N	O	S	0	0	0
			2042	1294	350	389	9			
1	D	255	Total	C	N	O	S	0	0	0
			2042	1294	350	389	9			
1	E	255	Total	C	N	O	S	0	0	0
			2042	1294	350	389	9			
1	F	255	Total	C	N	O	S	0	0	0
			2042	1294	350	389	9			
1	G	249	Total	C	N	O	S	0	0	0
			1884	1188	325	362	9			
1	H	255	Total	C	N	O	S	0	0	0
			2042	1294	350	389	9			
1	I	255	Total	C	N	O	S	0	0	0
			2042	1294	350	389	9			
1	J	255	Total	C	N	O	S	0	0	0
			2042	1294	350	389	9			
1	K	255	Total	C	N	O	S	0	0	0
			2042	1294	350	389	9			
1	L	255	Total	C	N	O	S	0	0	0
			2042	1294	350	389	9			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	EXPRESSION TAG	UNP Q8U3I4
A	1	VAL	-	EXPRESSION TAG	UNP Q8U3I4
B	0	SER	-	EXPRESSION TAG	UNP Q8U3I4
B	1	VAL	-	EXPRESSION TAG	UNP Q8U3I4
C	0	SER	-	EXPRESSION TAG	UNP Q8U3I4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1	VAL	-	EXPRESSION TAG	UNP Q8U3I4
D	0	SER	-	EXPRESSION TAG	UNP Q8U3I4
D	1	VAL	-	EXPRESSION TAG	UNP Q8U3I4
E	0	SER	-	EXPRESSION TAG	UNP Q8U3I4
E	1	VAL	-	EXPRESSION TAG	UNP Q8U3I4
F	0	SER	-	EXPRESSION TAG	UNP Q8U3I4
F	1	VAL	-	EXPRESSION TAG	UNP Q8U3I4
G	0	SER	-	EXPRESSION TAG	UNP Q8U3I4
G	1	VAL	-	EXPRESSION TAG	UNP Q8U3I4
H	0	SER	-	EXPRESSION TAG	UNP Q8U3I4
H	1	VAL	-	EXPRESSION TAG	UNP Q8U3I4
I	0	SER	-	EXPRESSION TAG	UNP Q8U3I4
I	1	VAL	-	EXPRESSION TAG	UNP Q8U3I4
J	0	SER	-	EXPRESSION TAG	UNP Q8U3I4
J	1	VAL	-	EXPRESSION TAG	UNP Q8U3I4
K	0	SER	-	EXPRESSION TAG	UNP Q8U3I4
K	1	VAL	-	EXPRESSION TAG	UNP Q8U3I4
L	0	SER	-	EXPRESSION TAG	UNP Q8U3I4
L	1	VAL	-	EXPRESSION TAG	UNP Q8U3I4

- Molecule 2 is a DNA chain called 30-mer oligo(dT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	7	Total	C	N	O	P	0	0	0
			141	70	14	50	7			
2	V	4	Total	C	N	O	P	0	0	0
			81	40	8	29	4			
2	Y	11	Total	C	N	O	P	0	0	0
			221	110	22	78	11			
2	Z	7	Total	C	N	O	P	0	0	0
			141	70	14	50	7			

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

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

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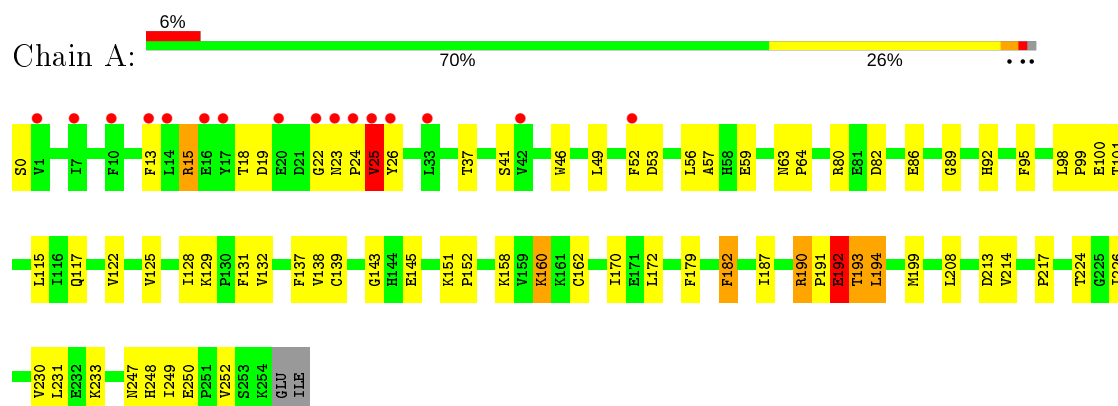
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	K	1	Total 1	Zn 1	0	0
3	E	1	Total 1	Zn 1	0	0
3	H	1	Total 1	Zn 1	0	0
3	B	1	Total 1	Zn 1	0	0
3	I	1	Total 1	Zn 1	0	0
3	C	1	Total 1	Zn 1	0	0
3	A	1	Total 1	Zn 1	0	0
3	L	1	Total 1	Zn 1	0	0
3	F	1	Total 1	Zn 1	0	0

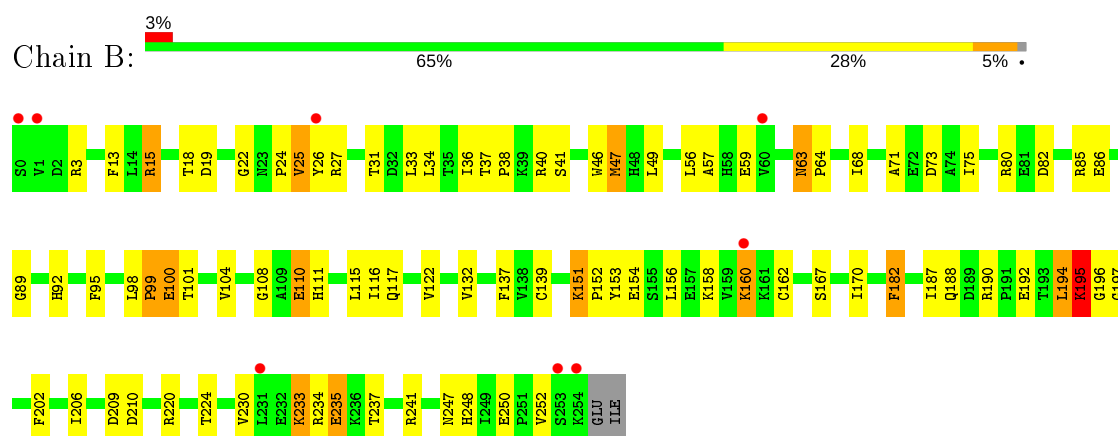
3 Residue-property plots [i](#)

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.

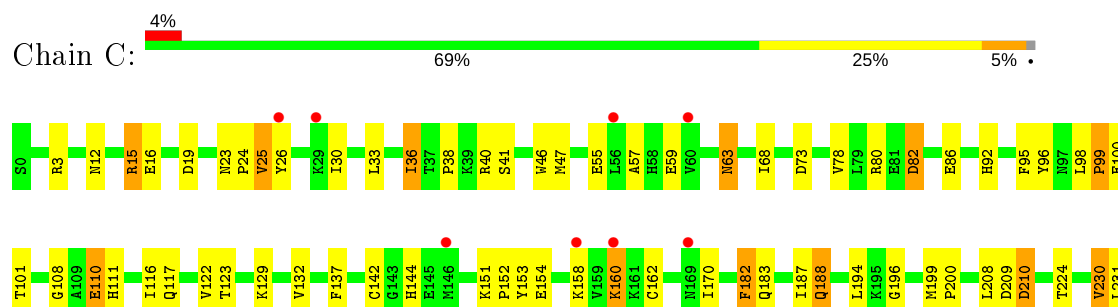
• Molecule 1: Cell division control protein 21



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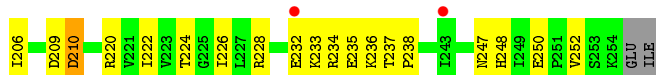




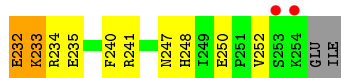
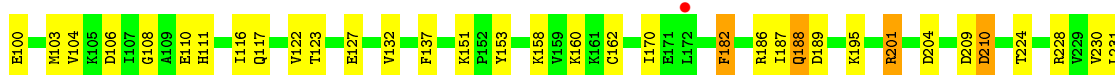
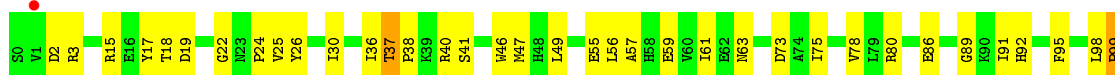
- Molecule 1: Cell division control protein 21



- Molecule 1: Cell division control protein 21

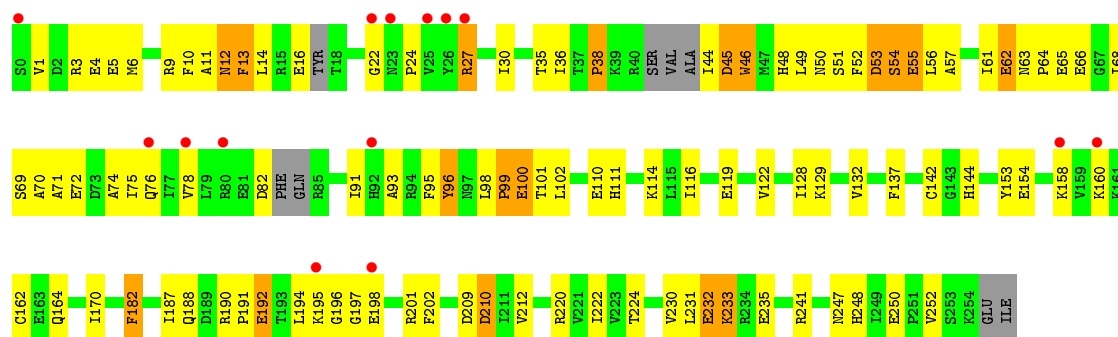


- Molecule 1: Cell division control protein 21

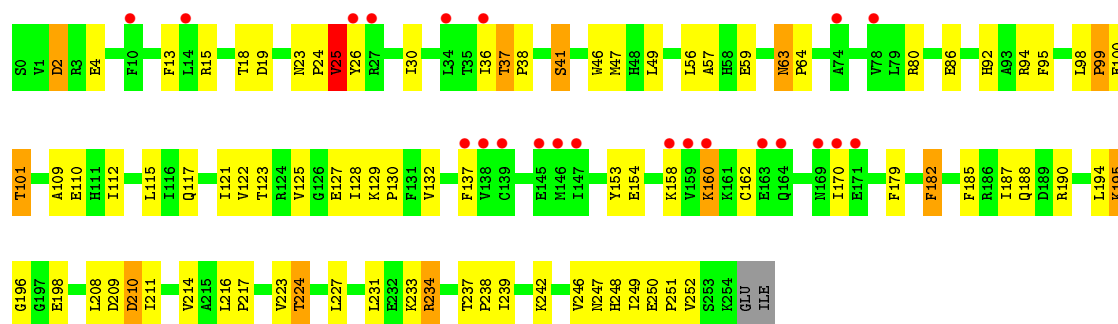


- Molecule 1: Cell division control protein 21

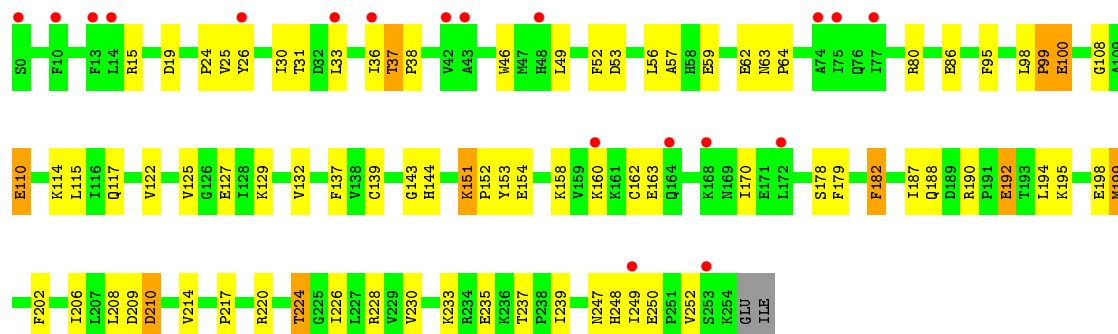




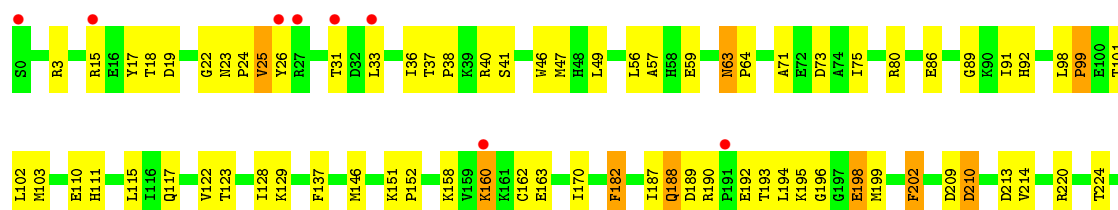
• Molecule 1: Cell division control protein 21

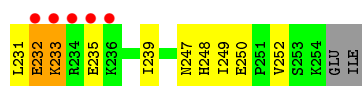


• Molecule 1: Cell division control protein 21

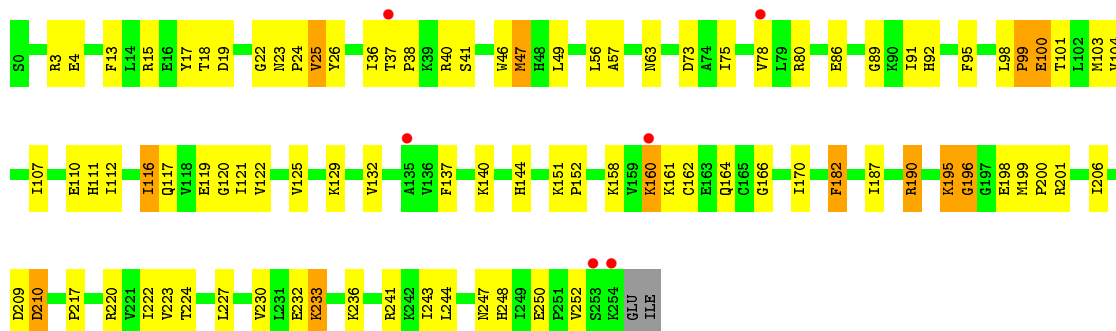


• Molecule 1: Cell division control protein 21

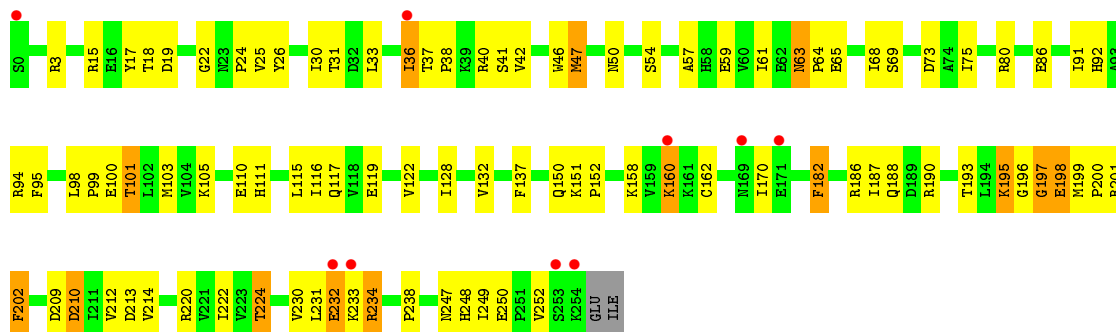




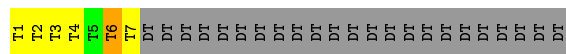
- Molecule 1: Cell division control protein 21



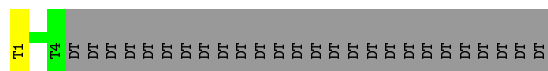
- Molecule 1: Cell division control protein 21



- Molecule 2: 30-mer oligo(dT)

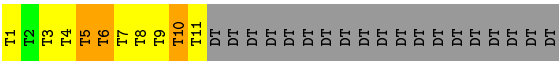


- Molecule 2: 30-mer oligo(dT)

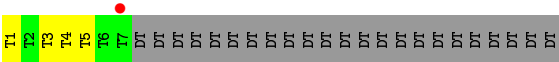


- Molecule 2: 30-mer oligo(dT)





● Molecule 2: 30-mer oligo(dT)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	94.28 Å 113.40 Å 196.85 Å 90.00° 101.35° 90.00°	Depositor
Resolution (Å)	48.51 – 3.20 48.52 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.51-3.20) 99.6 (48.52-3.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 3.19 Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.257 , 0.294 0.249 , 0.285	Depositor DCC
R_{free} test set	3376 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	81.0	Xtriage
Anisotropy	0.558	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 54.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.028 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	24942	wwPDB-VP
Average B, all atoms (Å ²)	129.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.41	0/2077	0.57	0/2805
1	B	0.40	0/2077	0.57	0/2805
1	C	0.39	0/2077	0.56	0/2805
1	D	0.42	0/2077	0.57	0/2805
1	E	0.39	0/2077	0.54	0/2805
1	F	0.39	0/2077	0.56	0/2805
1	G	0.41	0/1909	0.63	2/2579 (0.1%)
1	H	0.47	0/2077	0.62	0/2805
1	I	0.40	0/2077	0.55	0/2805
1	J	0.41	0/2077	0.55	0/2805
1	K	0.50	0/2077	0.65	0/2805
1	L	0.46	0/2077	0.61	0/2805
2	V	1.47	1/88 (1.1%)	1.48	0/132
2	X	1.15	1/154 (0.6%)	1.46	1/234 (0.4%)
2	Y	1.01	1/242 (0.4%)	1.57	5/370 (1.4%)
2	Z	1.15	1/154 (0.6%)	1.36	0/234
All	All	0.45	4/25394 (0.0%)	0.63	8/34404 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	V	1	DT	OP3-P	-11.02	1.48	1.61
2	X	1	DT	OP3-P	-10.94	1.48	1.61
2	Y	1	DT	OP3-P	-10.85	1.48	1.61
2	Z	1	DT	OP3-P	-10.85	1.48	1.61

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	6	DT	C4-C5-C7	6.18	122.71	119.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	10	DT	C4-C5-C7	6.08	122.65	119.00
1	G	24	PRO	N-CA-CB	5.96	110.45	103.30
1	G	38	PRO	N-CA-CB	5.72	110.16	103.30
2	Y	6	DT	C6-C5-C7	-5.52	119.59	122.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2042	0	2052	44	0
1	B	2042	0	2052	62	0
1	C	2042	0	2052	56	0
1	D	2042	0	2052	61	0
1	E	2042	0	2052	48	0
1	F	2042	0	2052	54	0
1	G	1884	0	1797	88	0
1	H	2042	0	2052	70	0
1	I	2042	0	2052	54	0
1	J	2042	0	2052	52	0
1	K	2042	0	2052	64	0
1	L	2042	0	2052	67	0
2	V	81	0	49	0	0
2	X	141	0	85	6	0
2	Y	221	0	133	14	0
2	Z	141	0	85	3	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	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
All	All	24942	0	24721	719	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.

The worst 5 of 719 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:X:6:DT:H2''	2:X:7:DT:H5''	1.46	0.97
1:L:41:SER:HB3	1:L:92:HIS:HB2	1.48	0.95
1:G:11:ALA:HA	1:G:14:LEU:HD12	1.51	0.93
1:G:72:GLU:O	1:G:75:ILE:HG22	1.74	0.87
1:I:188:GLN:HB3	1:I:202:PHE:HB3	1.56	0.87

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	253/257 (98%)	219 (87%)	26 (10%)	8 (3%)	4	26
1	B	253/257 (98%)	219 (87%)	26 (10%)	8 (3%)	4	26
1	C	253/257 (98%)	223 (88%)	25 (10%)	5 (2%)	7	38
1	D	253/257 (98%)	221 (87%)	26 (10%)	6 (2%)	6	34
1	E	253/257 (98%)	220 (87%)	26 (10%)	7 (3%)	5	29
1	F	253/257 (98%)	224 (88%)	24 (10%)	5 (2%)	7	38
1	G	241/257 (94%)	191 (79%)	38 (16%)	12 (5%)	2	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	253/257 (98%)	227 (90%)	21 (8%)	5 (2%)	7	38
1	I	253/257 (98%)	221 (87%)	26 (10%)	6 (2%)	6	34
1	J	253/257 (98%)	225 (89%)	23 (9%)	5 (2%)	7	38
1	K	253/257 (98%)	218 (86%)	29 (12%)	6 (2%)	6	34
1	L	253/257 (98%)	219 (87%)	27 (11%)	7 (3%)	5	29
All	All	3024/3084 (98%)	2627 (87%)	317 (10%)	80 (3%)	5	31

5 of 80 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	VAL
1	A	233	LYS
1	B	25	VAL
1	B	233	LYS
1	C	25	VAL

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	230/233 (99%)	216 (94%)	14 (6%)	18	54
1	B	230/233 (99%)	215 (94%)	15 (6%)	17	51
1	C	230/233 (99%)	213 (93%)	17 (7%)	13	46
1	D	230/233 (99%)	209 (91%)	21 (9%)	9	34
1	E	230/233 (99%)	217 (94%)	13 (6%)	20	56
1	F	230/233 (99%)	215 (94%)	15 (6%)	17	51
1	G	195/233 (84%)	177 (91%)	18 (9%)	9	33
1	H	230/233 (99%)	211 (92%)	19 (8%)	11	40
1	I	230/233 (99%)	216 (94%)	14 (6%)	18	54
1	J	230/233 (99%)	215 (94%)	15 (6%)	17	51
1	K	230/233 (99%)	210 (91%)	20 (9%)	10	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	230/233 (99%)	211 (92%)	19 (8%)	11	40
All	All	2725/2796 (98%)	2525 (93%)	200 (7%)	14	46

5 of 200 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	195	LYS
1	G	232	GLU
1	L	47	MET
1	F	232	GLU
1	G	65	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	12	ASN
1	G	58	HIS
1	K	247	ASN
1	G	48	HIS
1	G	188	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](#)

Of 12 ligands modelled in this entry, 12 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 ⓘ

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	255/257 (99%)	0.21	16 (6%) 20 11	65, 120, 219, 325	0
1	B	255/257 (99%)	0.13	8 (3%) 49 32	65, 113, 189, 316	0
1	C	255/257 (99%)	0.11	10 (3%) 39 25	74, 113, 192, 268	0
1	D	255/257 (99%)	0.08	11 (4%) 35 22	67, 112, 200, 251	0
1	E	255/257 (99%)	0.33	14 (5%) 25 14	69, 128, 219, 278	0
1	F	255/257 (99%)	0.02	4 (1%) 72 59	69, 116, 197, 270	0
1	G	249/257 (96%)	0.30	14 (5%) 24 13	75, 136, 219, 279	0
1	H	255/257 (99%)	0.39	22 (8%) 10 5	59, 117, 272, 410	0
1	I	255/257 (99%)	0.40	19 (7%) 14 8	75, 148, 274, 362	0
1	J	255/257 (99%)	0.22	13 (5%) 28 16	71, 119, 214, 329	0
1	K	255/257 (99%)	0.13	6 (2%) 59 44	60, 108, 191, 266	0
1	L	255/257 (99%)	0.14	9 (3%) 44 28	58, 102, 198, 344	0
2	V	4/30 (13%)	0.39	0 100 100	109, 118, 146, 179	0
2	X	7/30 (23%)	0.55	0 100 100	104, 139, 191, 219	0
2	Y	11/30 (36%)	0.47	0 100 100	163, 184, 240, 246	0
2	Z	7/30 (23%)	0.81	1 (14%) 2 1	138, 187, 215, 219	0
All	All	3083/3204 (96%)	0.21	147 (4%) 30 18	58, 119, 224, 410	0

The worst 5 of 147 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	159	VAL	10.6
1	L	253	SER	9.5
1	F	254	LYS	8.9
1	H	158	LYS	8.1
1	K	253	SER	7.1

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](#)

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(\AA^2)	Q<0.9
3	ZN	E	301	1/1	0.65	0.11	218,218,218,218	0
3	ZN	F	301	1/1	0.69	0.07	206,206,206,206	0
3	ZN	C	301	1/1	0.80	0.04	188,188,188,188	0
3	ZN	I	301	1/1	0.82	0.12	260,260,260,260	0
3	ZN	D	301	1/1	0.83	0.11	190,190,190,190	0
3	ZN	H	301	1/1	0.91	0.07	311,311,311,311	0
3	ZN	A	301	1/1	0.91	0.21	176,176,176,176	0
3	ZN	L	301	1/1	0.92	0.16	201,201,201,201	0
3	ZN	J	301	1/1	0.94	0.15	169,169,169,169	0
3	ZN	K	301	1/1	0.95	0.12	179,179,179,179	0
3	ZN	G	301	1/1	0.97	0.23	181,181,181,181	0
3	ZN	B	301	1/1	0.99	0.21	159,159,159,159	0

6.5 Other polymers [i](#)

There are no such residues in this entry.