



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 12, 2022 – 02:07 PM EDT

PDB ID : 7MW8  
Title : Crystal Structure Analysis of Xac Nucleotide Pyrophosphatase/Phosphodiesterase  
Authors : Fernandez, D.; Li, L.; Brown, J.A.  
Deposited on : 2021-05-15  
Resolution : 1.90 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.28.1
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)	:	2.28.1

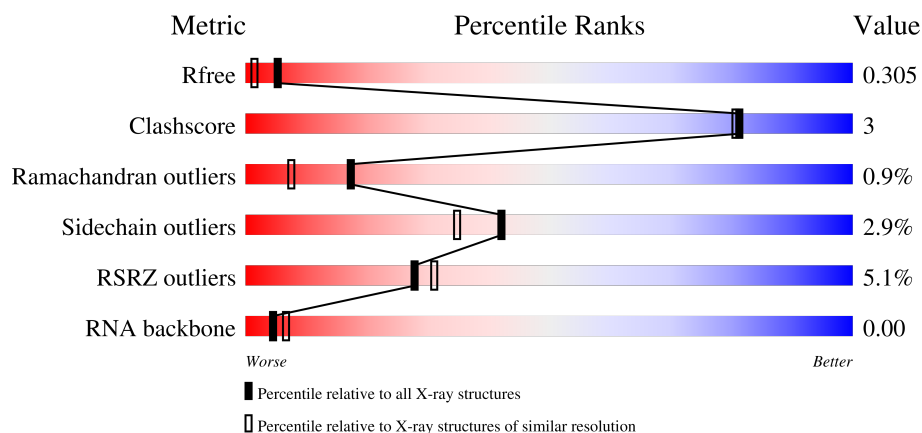
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)
RNA backbone	3102	1013 (2.42-1.38)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	427	<div> <div>5%</div> <div>81% 7% 11%</div> </div>
1	B	427	<div> <div>3%</div> <div>81% 8% 10%</div> </div>
1	C	427	<div> <div>2%</div> <div>83% 6% 10%</div> </div>
1	D	427	<div> <div>7%</div> <div>83% 7% 10%</div> </div>

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Mol	Chain	Length	Quality of chain
1	E	427	<div><div>8%</div><div><div></div><div>79%</div><div>9%</div><div>10%</div></div></div>
1	F	427	<div><div>3%</div><div><div></div><div>84%</div><div>6%</div><div>10%</div></div></div>
2	J	2	<div><div>50%</div><div><div></div><div>50%</div><div>50%</div></div></div>
2	K	2	<div><div>50%</div><div><div></div><div>50%</div></div></div>
2	L	2	<div><div>50%</div><div><div></div><div>50%</div></div></div>
2	M	2	<div><div>50%</div><div><div></div><div>50%</div></div></div>
2	N	2	<div><div>50%</div><div><div></div><div>50%</div></div></div>
2	O	2	<div><div>50%</div><div><div></div><div>50%</div></div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18189 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 Phosphodiesterase-nucleotide pyrophosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	383	Total	C	N	O	S	0	1	0
			2921	1838	543	529	11			
1	B	384	Total	C	N	O	S	0	0	0
			2943	1851	549	532	11			
1	C	385	Total	C	N	O	S	0	0	0
			2943	1850	549	533	11			
1	A	380	Total	C	N	O	S	0	1	0
			2908	1830	542	525	11			
1	E	384	Total	C	N	O	S	0	1	0
			2942	1851	550	530	11			
1	F	384	Total	C	N	O	S	0	1	0
			2960	1858	554	537	11			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	90	ALA	THR	engineered mutation	UNP A0A0U5FM15
B	90	ALA	THR	engineered mutation	UNP A0A0U5FM15
C	90	ALA	THR	engineered mutation	UNP A0A0U5FM15
A	90	ALA	THR	engineered mutation	UNP A0A0U5FM15
E	90	ALA	THR	engineered mutation	UNP A0A0U5FM15
F	90	ALA	THR	engineered mutation	UNP A0A0U5FM15

- Molecule 2 is a RNA chain called pApG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	J	2	Total	C	N	O	P	0	0	0
			46	20	10	14	2			
2	K	1	Total	C	N	O	P	0	0	0
			23	10	5	7	1			
2	L	1	Total	C	N	O	P	0	0	0
			23	10	5	7	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	1	Total	C	N	O	P	0	0	0
			23	10	5	7	1			
2	N	1	Total	C	N	O	P	0	0	0
			23	10	5	7	1			
2	O	1	Total	C	N	O	P	0	0	0
			23	10	5	7	1			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	2	Total	Zn	0	0
			2	2		
3	B	2	Total	Zn	0	0
			2	2		
3	C	2	Total	Zn	0	0
			2	2		
3	A	2	Total	Zn	0	0
			2	2		
3	E	2	Total	Zn	0	0
			2	2		
3	F	2	Total	Zn	0	0
			2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	46	Total	O	0	0
			46	46		
4	B	74	Total	O	0	0
			74	74		
4	C	73	Total	O	0	0
			73	73		
4	A	69	Total	O	0	0
			69	69		
4	E	53	Total	O	0	0
			53	53		
4	F	75	Total	O	0	0
			75	75		
4	J	3	Total	O	0	0
			3	3		
4	L	2	Total	O	0	0
			2	2		

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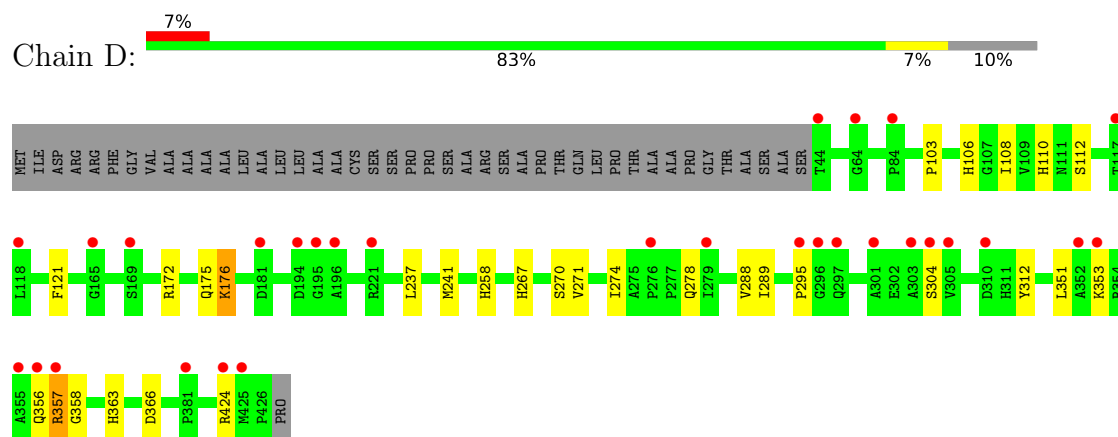
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	M	2	Total 2	O 2	0	0
4	N	1	Total 1	O 1	0	0
4	O	1	Total 1	O 1	0	0

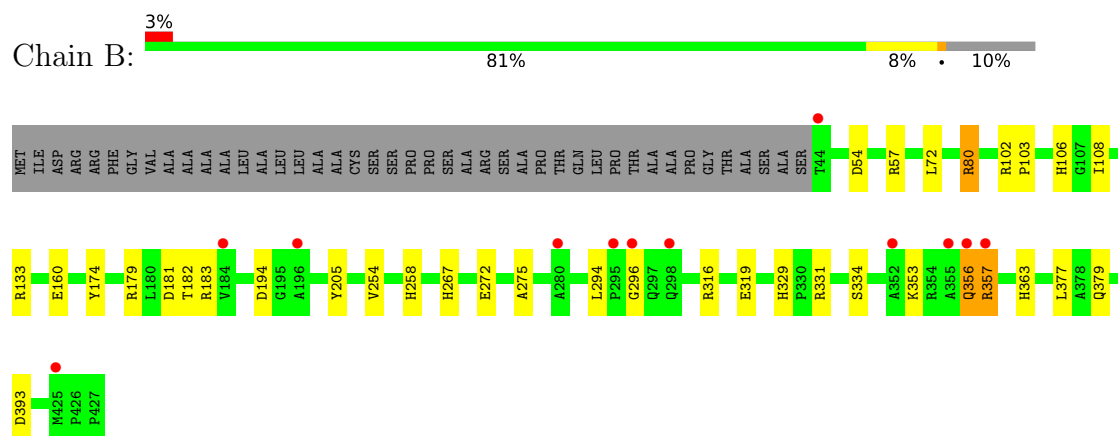
### 3 Residue-property plots [i](#)

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.

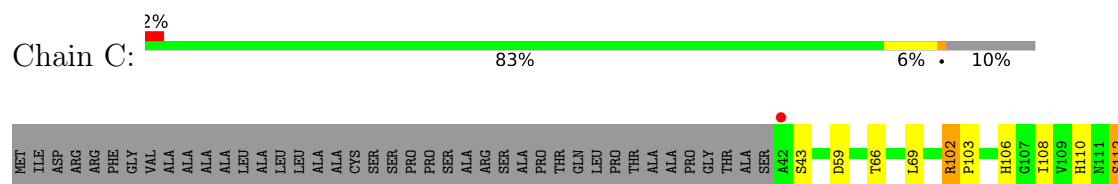
- Molecule 1: Phosphodiesterase-nucleotide pyrophosphatase

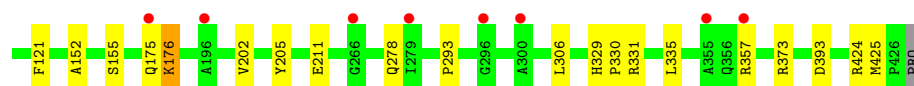


- Molecule 1: Phosphodiesterase-nucleotide pyrophosphatase

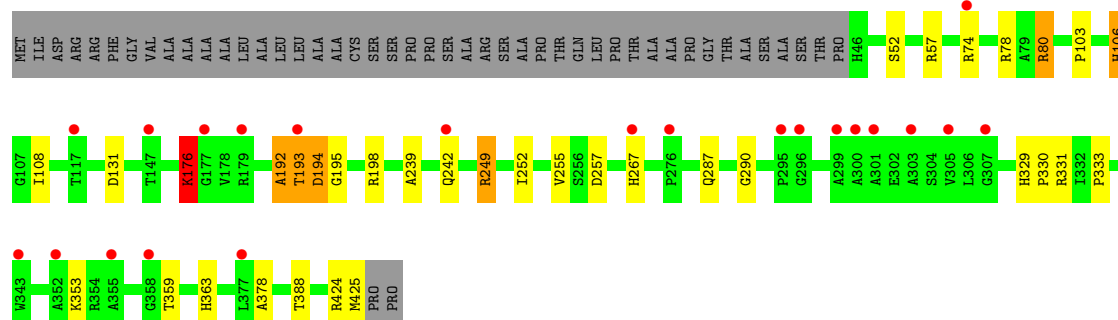
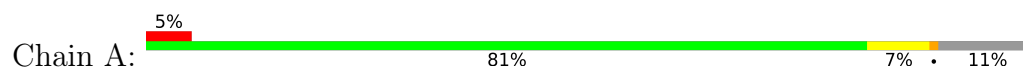


- Molecule 1: Phosphodiesterase-nucleotide pyrophosphatase

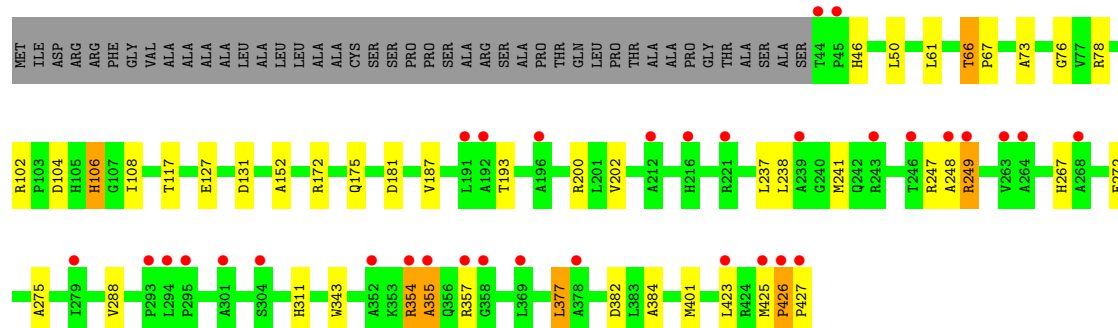
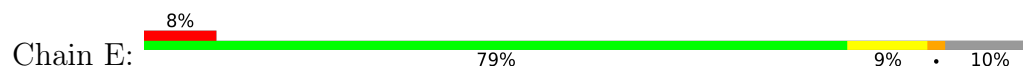




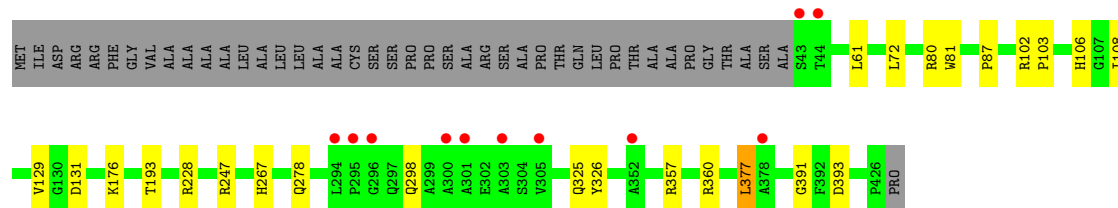
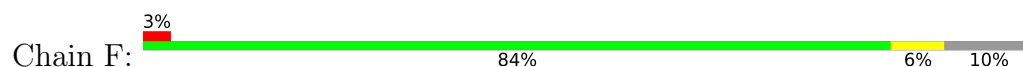
- Molecule 1: Phosphodiesterase-nucleotide pyrophosphatase



- Molecule 1: Phosphodiesterase-nucleotide pyrophosphatase



- Molecule 1: Phosphodiesterase-nucleotide pyrophosphatase



- Molecule 2: pApG





## ● Molecule 2: pApG

Chain K:  50% 50% A1 G

## ● Molecule 2: pApG

Chain L:  50% 50% A1 G

## ● Molecule 2: pApG

Chain M:  50% 50% A1 G

## ● Molecule 2: pApG

Chain N:  50% 50% A1 G

## ● Molecule 2: pApG

Chain O:  50% 50% A1 G

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	130.42Å 66.72Å 134.96Å 90.00° 116.25° 90.00°	Depositor
Resolution (Å)	30.04 – 1.90 38.99 – 1.90	Depositor EDS
% Data completeness (in resolution range)	94.5 (30.04-1.90) 94.5 (38.99-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.65 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.243 , 0.303 0.249 , 0.305	Depositor DCC
$R_{free}$ test set	7565 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.6	Xtriage
Anisotropy	0.761	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 33.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.036 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	18189	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	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 50.81 % 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 6.1311e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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	0.67	0/2995	0.83	2/4088 (0.0%)
1	B	0.70	0/3030	0.88	6/4138 (0.1%)
1	C	0.65	0/3029	0.84	3/4136 (0.1%)
1	D	0.61	0/3010	0.80	1/4112 (0.0%)
1	E	0.67	0/3029	0.86	4/4137 (0.1%)
1	F	0.67	0/3046	0.84	4/4157 (0.1%)
2	J	4.31	12/51 (23.5%)	6.32	20/76 (26.3%)
2	K	4.34	7/25 (28.0%)	6.26	11/35 (31.4%)
2	L	3.89	4/25 (16.0%)	6.88	12/35 (34.3%)
2	M	3.68	5/25 (20.0%)	7.13	13/35 (37.1%)
2	N	4.34	6/25 (24.0%)	6.73	10/35 (28.6%)
2	O	4.65	7/25 (28.0%)	5.88	9/35 (25.7%)
All	All	0.78	41/18315 (0.2%)	1.06	95/25019 (0.4%)

The worst 5 of 41 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	1	A	C5-C4	13.30	1.48	1.38
2	J	2	G	C5-C4	13.02	1.47	1.38
2	K	1	A	C5-C4	11.03	1.46	1.38
2	N	1	A	N7-C5	-10.70	1.32	1.39
2	J	1	A	C5-C4	10.34	1.46	1.38

The worst 5 of 95 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	1	A	C2-N3-C4	26.20	123.70	110.60
2	L	1	A	C2-N3-C4	24.63	122.92	110.60
2	K	1	A	C2-N3-C4	22.16	121.68	110.60
2	N	1	A	C2-N3-C4	20.78	120.99	110.60
2	O	1	A	C2-N3-C4	20.73	120.97	110.60

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	2908	0	2807	21	0
1	B	2943	0	2846	13	0
1	C	2943	0	2843	13	0
1	D	2921	0	2809	13	0
1	E	2942	0	2844	21	0
1	F	2960	0	2864	11	0
2	J	46	0	23	1	0
2	K	23	0	12	1	0
2	L	23	0	12	0	0
2	M	23	0	12	0	0
2	N	23	0	12	0	0
2	O	23	0	12	1	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
4	A	69	0	0	0	0
4	B	74	0	0	0	0
4	C	73	0	0	0	0
4	D	46	0	0	1	0
4	E	53	0	0	0	0
4	F	75	0	0	0	0
4	J	3	0	0	0	0
4	L	2	0	0	0	0
4	M	2	0	0	0	0
4	N	1	0	0	0	0
4	O	1	0	0	1	0
All	All	18189	0	17096	92	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 3.

The worst 5 of 92 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:A:80[B]:ARG:HG3	1:A:80[B]:ARG:NH1	1.59	1.03
1:A:80[B]:ARG:HG3	1:A:80[B]:ARG:HH11	0.91	1.03
1:A:80[B]:ARG:HH11	1:A:80[B]:ARG:CG	1.73	1.02
1:E:106:HIS:HD2	1:E:108:ILE:H	1.39	0.70
1:E:187:VAL:HG13	1:E:202:VAL:HG11	1.79	0.65

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	379/427 (89%)	356 (94%)	18 (5%)	5 (1%)	12	4
1	B	382/427 (90%)	369 (97%)	10 (3%)	3 (1%)	19	9
1	C	383/427 (90%)	367 (96%)	13 (3%)	3 (1%)	19	9
1	D	382/427 (90%)	363 (95%)	15 (4%)	4 (1%)	15	6
1	E	383/427 (90%)	359 (94%)	20 (5%)	4 (1%)	15	6
1	F	383/427 (90%)	372 (97%)	10 (3%)	1 (0%)	41	31
All	All	2292/2562 (90%)	2186 (95%)	86 (4%)	20 (1%)	17	7

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	357	ARG
1	A	176	LYS
1	A	194	ASP
1	E	248	ALA
1	E	354	ARG

### 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	290/326 (89%)	279 (96%)	11 (4%)	33	24
1	B	296/326 (91%)	289 (98%)	7 (2%)	49	43
1	C	295/326 (90%)	289 (98%)	6 (2%)	55	51
1	D	291/326 (89%)	285 (98%)	6 (2%)	53	48
1	E	295/326 (90%)	281 (95%)	14 (5%)	26	16
1	F	299/326 (92%)	290 (97%)	9 (3%)	41	33
All	All	1766/1956 (90%)	1713 (97%)	53 (3%)	42	33

5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	424	ARG
1	E	172	ARG
1	F	298	GLN
1	A	425	MET
1	E	106	HIS

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

Mol	Chain	Res	Type
1	A	329	HIS
1	E	267	HIS
1	E	242	GLN
1	E	329	HIS
1	B	267	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	J	1/2 (50%)	0	0
2	K	0/2	-	-

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	L	0/2	-	-
2	M	0/2	-	-
2	N	0/2	-	-
2	O	0/2	-	-
All	All	1/12 (8%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

## 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 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 [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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	380/427 (88%)	0.55	22 (5%) 23 25	22, 36, 59, 74	0
1	B	384/427 (89%)	0.16	12 (3%) 49 51	18, 31, 58, 78	0
1	C	385/427 (90%)	0.16	9 (2%) 60 63	19, 33, 59, 72	0
1	D	383/427 (89%)	0.64	30 (7%) 13 14	28, 42, 68, 84	0
1	E	384/427 (89%)	0.70	33 (8%) 10 12	21, 40, 64, 82	0
1	F	384/427 (89%)	0.24	11 (2%) 51 54	21, 32, 53, 65	0
2	J	2/2 (100%)	0.95	1 (50%) 0 0	31, 31, 31, 62	0
2	K	1/2 (50%)	-0.58	0 100 100	37, 37, 37, 37	0
2	L	1/2 (50%)	-0.60	0 100 100	25, 25, 25, 25	0
2	M	1/2 (50%)	-0.44	0 100 100	27, 27, 27, 27	0
2	N	1/2 (50%)	-0.27	0 100 100	35, 35, 35, 35	0
2	O	1/2 (50%)	-0.14	0 100 100	34, 34, 34, 34	0
All	All	2307/2574 (89%)	0.41	118 (5%) 28 31	18, 35, 61, 84	0

The worst 5 of 118 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	299	ALA	6.1
1	F	303	ALA	6.1
1	E	301	ALA	5.9
1	A	177	GLY	5.8
1	E	358	GLY	5.7

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	ZN	A	502	1/1	0.98	0.04	26,26,26,26	0
3	ZN	E	501	1/1	0.98	0.06	37,37,37,37	0
3	ZN	A	501	1/1	0.99	0.04	26,26,26,26	0
3	ZN	D	502	1/1	0.99	0.05	32,32,32,32	0
3	ZN	B	502	1/1	0.99	0.06	24,24,24,24	0
3	ZN	E	502	1/1	0.99	0.04	33,33,33,33	0
3	ZN	B	501	1/1	1.00	0.05	21,21,21,21	0
3	ZN	D	501	1/1	1.00	0.04	29,29,29,29	0
3	ZN	C	501	1/1	1.00	0.04	24,24,24,24	0
3	ZN	C	502	1/1	1.00	0.06	24,24,24,24	0
3	ZN	F	501	1/1	1.00	0.07	26,26,26,26	0
3	ZN	F	502	1/1	1.00	0.05	28,28,28,28	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.