



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 07:29 am GMT

PDB ID : 4LY6  
Title : Nucleotide-induced asymmetry within ATPase activator ring drives s54-RNAP interaction and ATP hydrolysis  
Authors : Sysoeva, T.A.; Chowdhury, S.; Guo, L.; Nixon, B.T.  
Deposited on : 2013-07-30  
Resolution : 3.60 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

<http://wwpdb.org/validation/2016/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  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

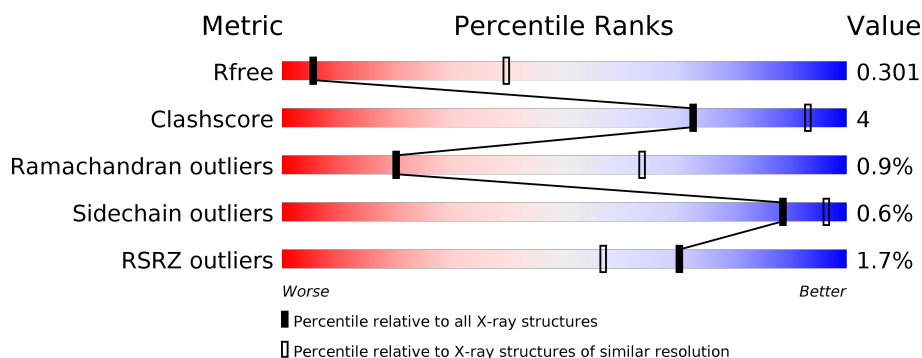
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.60 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))
$R_{free}$	100719	1026 (3.74-3.46)
Clashscore	112137	1036 (3.70-3.50)
Ramachandran outliers	110173	1030 (3.72-3.48)
Sidechain outliers	110143	1030 (3.72-3.48)
RSRZ outliers	101464	1051 (3.74-3.46)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	268	<div> <div>%</div> <div> <div></div> <div>84%</div> <div>9%</div> <div>8%</div> </div> </div>
1	B	268	<div> <div>%</div> <div> <div></div> <div>85%</div> <div>7%</div> <div>8%</div> </div> </div>
1	C	268	<div> <div>%</div> <div> <div></div> <div>84%</div> <div>9%</div> <div>8%</div> </div> </div>
1	D	268	<div> <div></div> <div> <div>80%</div> <div>11%</div> <div>8%</div> </div> </div>
1	E	268	<div> <div></div> <div> <div>83%</div> <div>9%</div> <div>8%</div> </div> </div>
1	F	268	<div> <div>%</div> <div> <div></div> <div>81%</div> <div>10%</div> <div>8%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	268	
1	H	268	
1	I	268	
1	J	268	
1	K	268	
1	L	268	
1	M	268	
1	N	268	
1	O	268	
1	P	268	
1	Q	268	
1	R	268	
1	S	268	
1	T	268	
1	U	268	
1	V	268	
1	W	268	
1	X	268	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 97439 atoms, of which 49249 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 Transcriptional regulator (NtrC family).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	247	Total	C	H	N	O	S	0	0	0
			4020	1278	2041	333	364	4			
1	B	247	Total	C	H	N	O	S	0	0	0
			4021	1278	2042	333	364	4			
1	C	247	Total	C	H	N	O	S	0	0	0
			4021	1278	2042	333	364	4			
1	D	247	Total	C	H	N	O	S	0	0	0
			4021	1278	2042	333	364	4			
1	E	247	Total	C	H	N	O	S	0	0	0
			4021	1278	2042	333	364	4			
1	F	247	Total	C	H	N	O	S	0	0	0
			4021	1278	2042	333	364	4			
1	G	247	Total	C	H	N	O	S	0	0	0
			4021	1278	2042	333	364	4			
1	H	247	Total	C	H	N	O	S	0	0	0
			4021	1278	2042	333	364	4			
1	I	247	Total	C	H	N	O	S	0	0	0
			4020	1278	2041	333	364	4			
1	J	247	Total	C	H	N	O	S	0	0	0
			4021	1278	2042	333	364	4			
1	K	247	Total	C	H	N	O	S	0	0	0
			4021	1278	2042	333	364	4			
1	L	247	Total	C	H	N	O	S	0	0	0
			4021	1278	2042	333	364	4			
1	M	247	Total	C	H	N	O	S	0	0	0
			4021	1278	2042	333	364	4			
1	N	247	Total	C	H	N	O	S	0	0	0
			4021	1278	2042	333	364	4			
1	O	247	Total	C	H	N	O	S	0	0	0
			4021	1278	2042	333	364	4			
1	P	247	Total	C	H	N	O	S	0	0	0
			4021	1278	2042	333	364	4			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	Q	247	Total	C	H	N	O	S	0	0	0
			4021	1278	2042	333	364	4			
1	R	247	Total	C	H	N	O	S	0	0	0
			4021	1278	2042	333	364	4			
1	S	247	Total	C	H	N	O	S	0	0	0
			4021	1278	2042	333	364	4			
1	T	247	Total	C	H	N	O	S	0	0	0
			4020	1278	2041	333	364	4			
1	U	247	Total	C	H	N	O	S	0	0	0
			4021	1278	2042	333	364	4			
1	V	247	Total	C	H	N	O	S	0	0	0
			4021	1278	2042	333	364	4			
1	W	247	Total	C	H	N	O	S	0	0	0
			4021	1278	2042	333	364	4			
1	X	247	Total	C	H	N	O	S	0	0	0
			4021	1278	2042	333	364	4			

There are 24 discrepancies between the modelled and reference sequences:

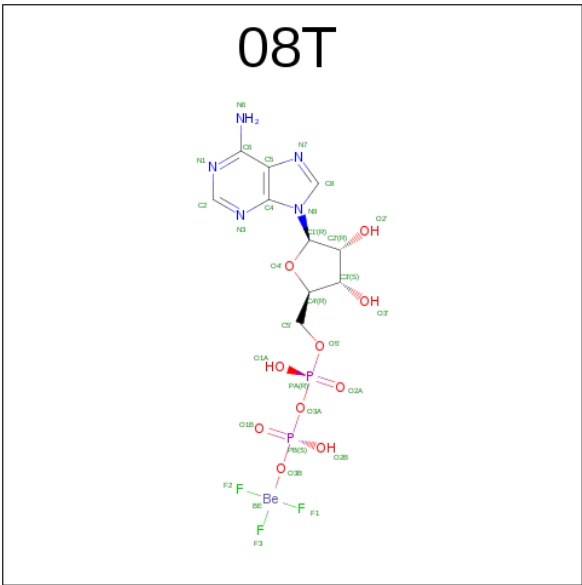
Chain	Residue	Modelled	Actual	Comment	Reference
A	120	MET	-	INITIATING METHIONINE	UNP O67198
B	120	MET	-	INITIATING METHIONINE	UNP O67198
C	120	MET	-	INITIATING METHIONINE	UNP O67198
D	120	MET	-	INITIATING METHIONINE	UNP O67198
E	120	MET	-	INITIATING METHIONINE	UNP O67198
F	120	MET	-	INITIATING METHIONINE	UNP O67198
G	120	MET	-	INITIATING METHIONINE	UNP O67198
H	120	MET	-	INITIATING METHIONINE	UNP O67198
I	120	MET	-	INITIATING METHIONINE	UNP O67198
J	120	MET	-	INITIATING METHIONINE	UNP O67198
K	120	MET	-	INITIATING METHIONINE	UNP O67198
L	120	MET	-	INITIATING METHIONINE	UNP O67198
M	120	MET	-	INITIATING METHIONINE	UNP O67198
N	120	MET	-	INITIATING METHIONINE	UNP O67198
O	120	MET	-	INITIATING METHIONINE	UNP O67198
P	120	MET	-	INITIATING METHIONINE	UNP O67198
Q	120	MET	-	INITIATING METHIONINE	UNP O67198
R	120	MET	-	INITIATING METHIONINE	UNP O67198
S	120	MET	-	INITIATING METHIONINE	UNP O67198
T	120	MET	-	INITIATING METHIONINE	UNP O67198
U	120	MET	-	INITIATING METHIONINE	UNP O67198
V	120	MET	-	INITIATING METHIONINE	UNP O67198
W	120	MET	-	INITIATING METHIONINE	UNP O67198

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Chain	Residue	Modelled	Actual	Comment	Reference
X	120	MET	-	INITIATING METHIONINE	UNP O67198

- Molecule 2 is [(((2R,3S,4R,5R)-5-(6-AMINOPURIN-9-YL)-3,4-BIS(OXIDANYL)OXOLAN-2-YL]METHOXY-OXIDANYL-PHOSPHORYL]OXY-OXIDANYL-PHOSPHORYL]OXY-TRIS(FLUORANYL)BERYLLIUM (three-letter code: 08T) (formula: C<sub>10</sub>H<sub>14</sub>BeF<sub>3</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms								ZeroOcc	AltConf
2	A	1	Total	Be	C	F	H	N	O	P	0	0
			42	1	10	3	11	5	10	2		
2	B	1	Total	Be	C	F	H	N	O	P	0	0
			42	1	10	3	11	5	10	2		
2	C	1	Total	Be	C	F	H	N	O	P	0	0
			42	1	10	3	11	5	10	2		
2	D	1	Total	Be	C	F	H	N	O	P	0	0
			42	1	10	3	11	5	10	2		
2	E	1	Total	Be	C	F	H	N	O	P	0	0
			42	1	10	3	11	5	10	2		
2	G	1	Total	Be	C	F	H	N	O	P	0	0
			42	1	10	3	11	5	10	2		
2	H	1	Total	Be	C	F	H	N	O	P	0	0
			42	1	10	3	11	5	10	2		
2	I	1	Total	Be	C	F	H	N	O	P	0	0
			42	1	10	3	11	5	10	2		
2	J	1	Total	Be	C	F	H	N	O	P	0	0
			42	1	10	3	11	5	10	2		

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Mol	Chain	Residues	Atoms								ZeroOcc	AltConf
2	K	1	Total	Be	C	F	H	N	O	P	0	0
			42	1	10	3	11	5	10	2		
2	M	1	Total	Be	C	F	H	N	O	P	0	0
			42	1	10	3	11	5	10	2		
2	N	1	Total	Be	C	F	H	N	O	P	0	0
			42	1	10	3	11	5	10	2		
2	O	1	Total	Be	C	F	H	N	O	P	0	0
			42	1	10	3	11	5	10	2		
2	P	1	Total	Be	C	F	H	N	O	P	0	0
			42	1	10	3	11	5	10	2		
2	Q	1	Total	Be	C	F	H	N	O	P	0	0
			42	1	10	3	11	5	10	2		
2	S	1	Total	Be	C	F	H	N	O	P	0	0
			42	1	10	3	11	5	10	2		
2	T	1	Total	Be	C	F	H	N	O	P	0	0
			42	1	10	3	11	5	10	2		
2	U	1	Total	Be	C	F	H	N	O	P	0	0
			42	1	10	3	11	5	10	2		
2	V	1	Total	Be	C	F	H	N	O	P	0	0
			42	1	10	3	11	5	10	2		
2	W	1	Total	Be	C	F	H	N	O	P	0	0
			42	1	10	3	11	5	10	2		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

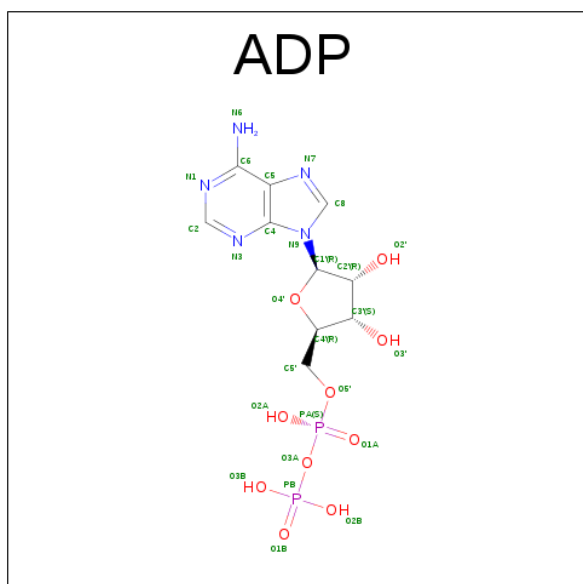
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	P	1	Total	Mg	0	0
			1	1		
3	G	1	Total	Mg	0	0
			1	1		
3	J	1	Total	Mg	0	0
			1	1		
3	Q	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	K	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	H	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Mg 1	0	0
3	I	1	Total 1	Mg 1	0	0
3	C	1	Total 1	Mg 1	0	0
3	V	1	Total 1	Mg 1	0	0
3	W	1	Total 1	Mg 1	0	0
3	A	1	Total 1	Mg 1	0	0
3	T	1	Total 1	Mg 1	0	0
3	N	1	Total 1	Mg 1	0	0
3	U	1	Total 1	Mg 1	0	0
3	O	1	Total 1	Mg 1	0	0
3	S	1	Total 1	Mg 1	0	0
3	M	1	Total 1	Mg 1	0	0

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



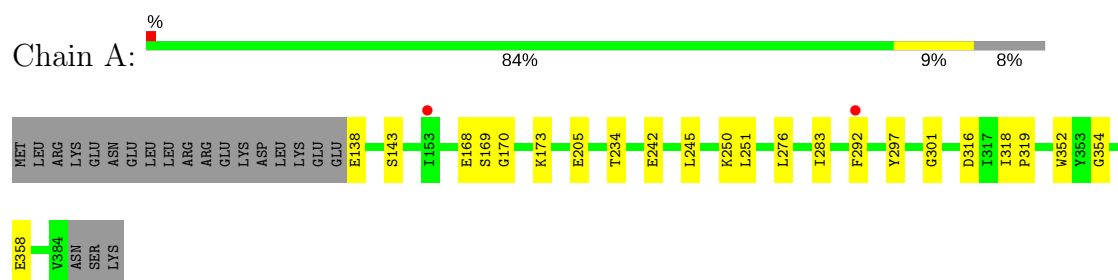


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	L	1	Total	C	H	N	O	P	0	0
			39	10	12	5	10	2		
4	X	1	Total	C	H	N	O	P	0	0
			39	10	12	5	10	2		

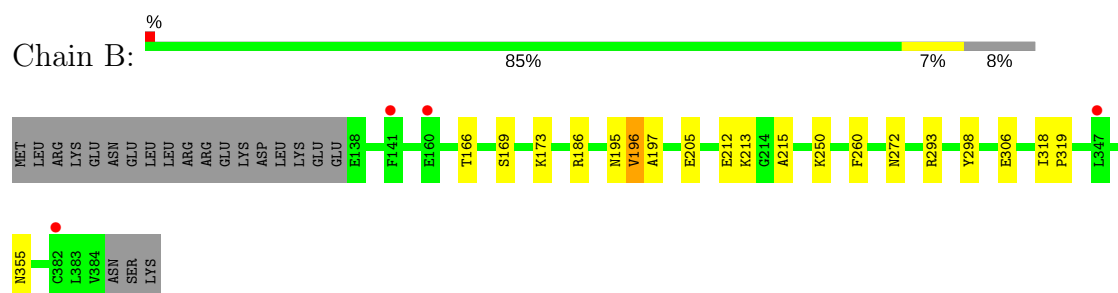
### 3 Residue-property plots [i](#)

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.

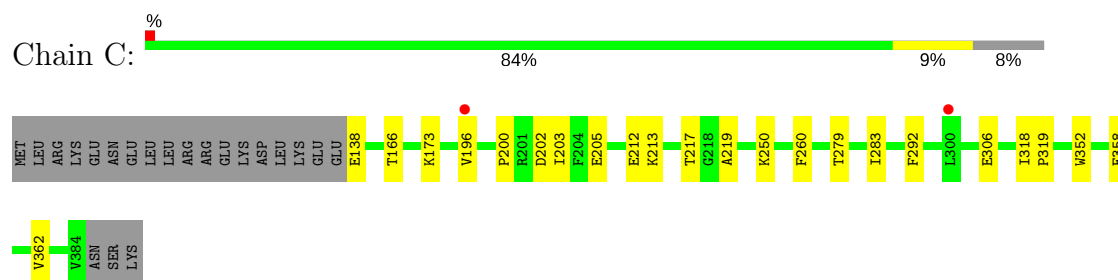
- Molecule 1: Transcriptional regulator (NtrC family)



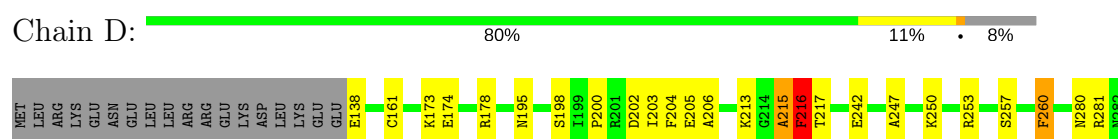
- Molecule 1: Transcriptional regulator (NtrC family)



- Molecule 1: Transcriptional regulator (NtrC family)



- Molecule 1: Transcriptional regulator (NtrC family)





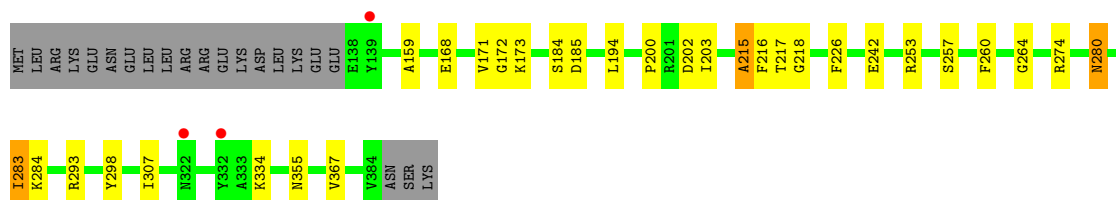
- Molecule 1: Transcriptional regulator (NtrC family)

Chain E: 83% 9% 8%



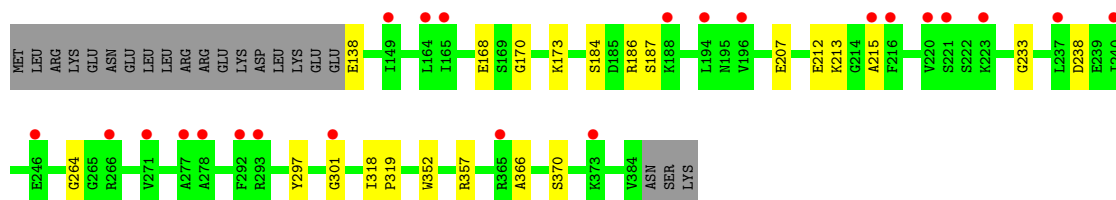
- Molecule 1: Transcriptional regulator (NtrC family)

Chain F: 81% 10% 8%



- Molecule 1: Transcriptional regulator (NtrC family)

Chain G: 9% 84% 8%



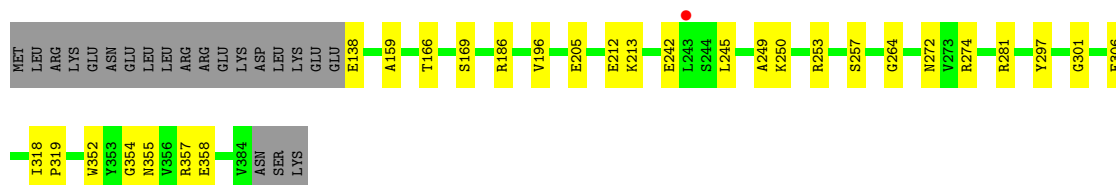
- Molecule 1: Transcriptional regulator (NtrC family)

Chain H: 85% 7% 8%

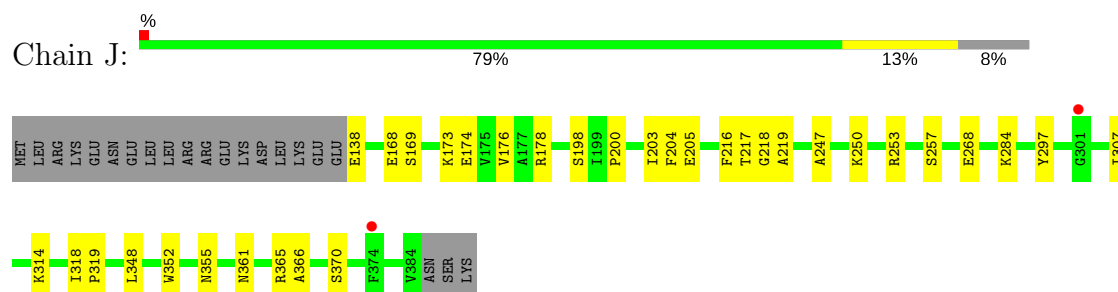


- Molecule 1: Transcriptional regulator (NtrC family)

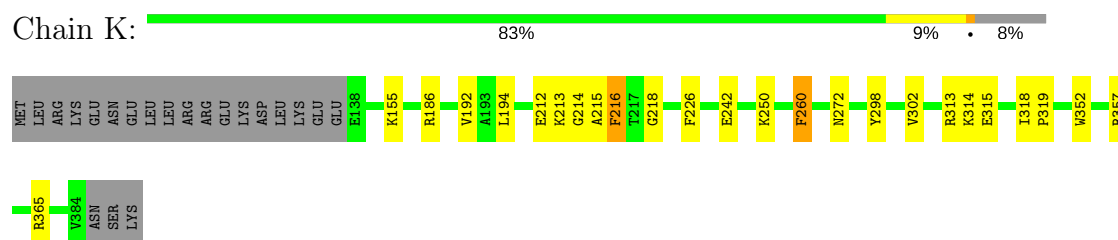
Chain I: 81% 11% 8%



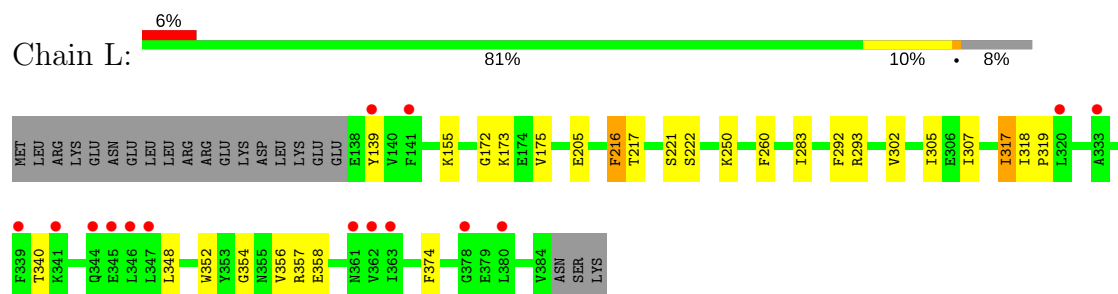
- Molecule 1: Transcriptional regulator (NtrC family)



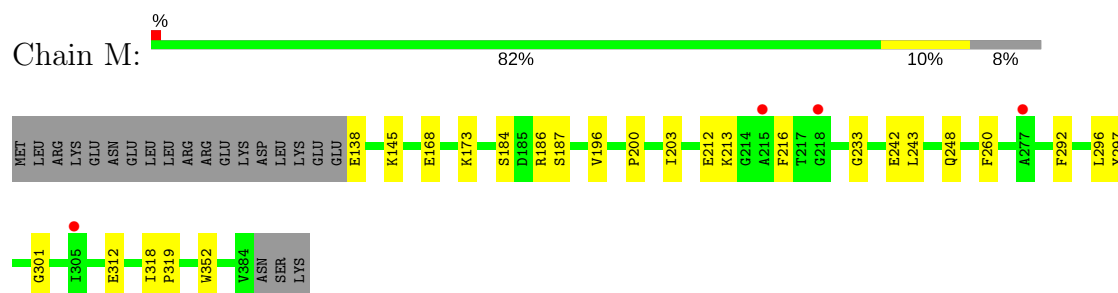
- Molecule 1: Transcriptional regulator (NtrC family)



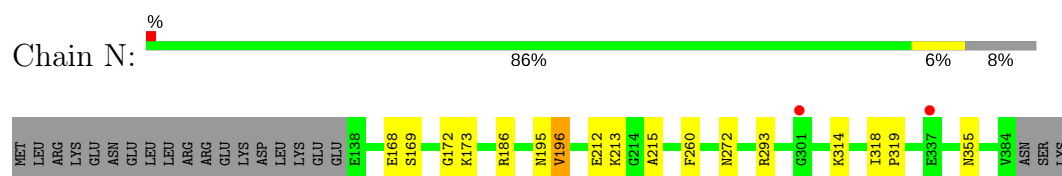
- Molecule 1: Transcriptional regulator (NtrC family)




- Molecule 1: Transcriptional regulator (NtrC family)

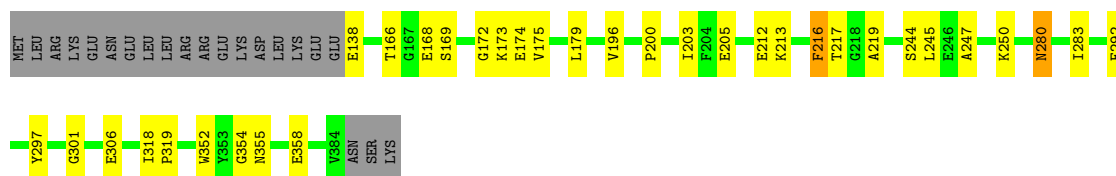


- Molecule 1: Transcriptional regulator (NtrC family)




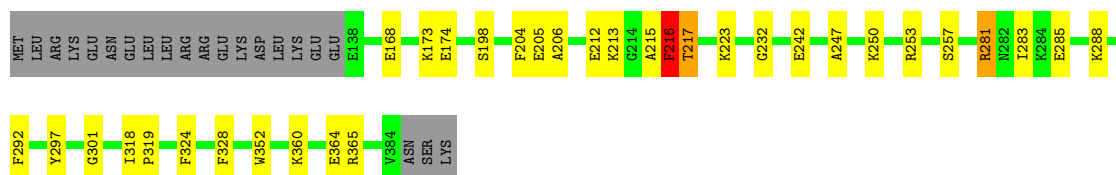
- Molecule 1: Transcriptional regulator (NtrC family)

Chain O:  79% 12% 8%




- Molecule 1: Transcriptional regulator (NtrC family)

Chain P:  79% 12% 8%




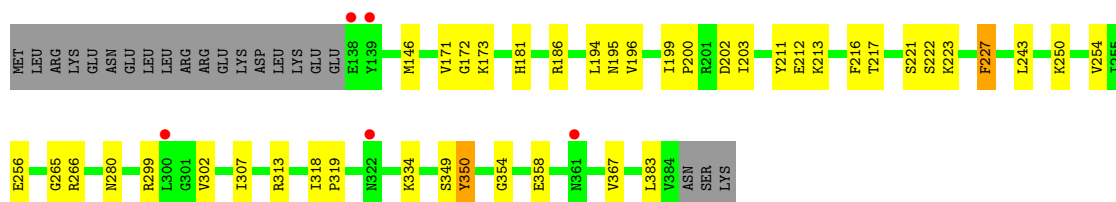
- Molecule 1: Transcriptional regulator (NtrC family)

Chain Q:  82% 10% 8%




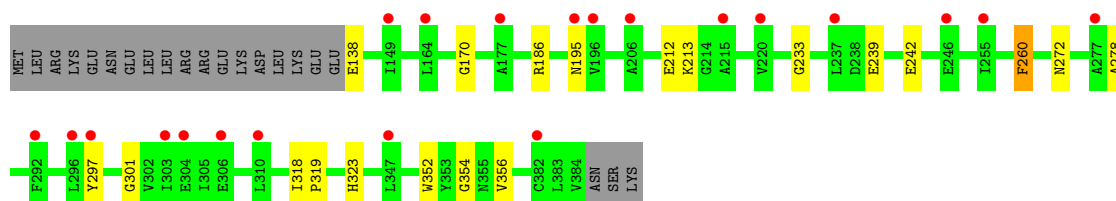
- Molecule 1: Transcriptional regulator (NtrC family)

Chain R:  2% 76% 15% 8%

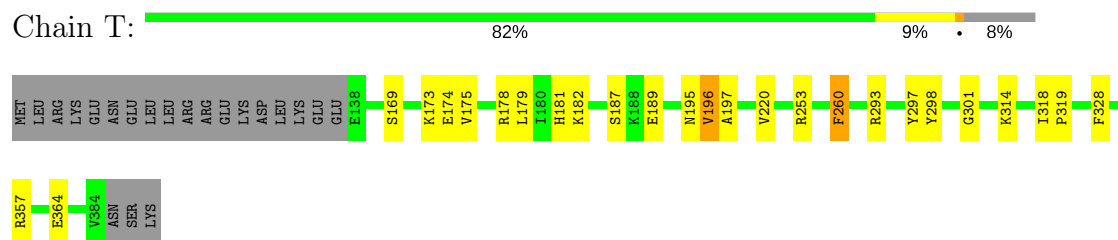


- Molecule 1: Transcriptional regulator (NtrC family)

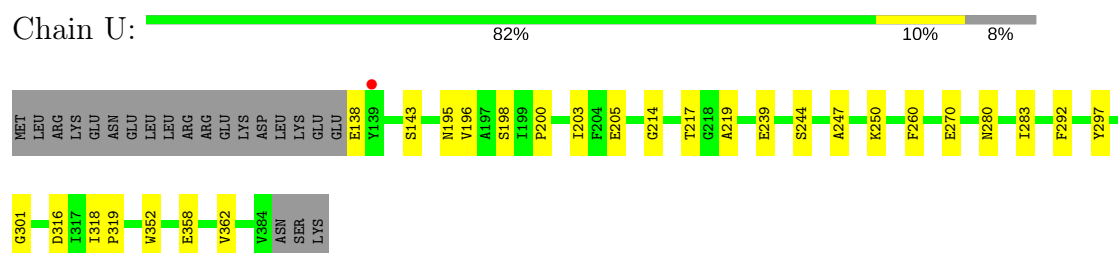
Chain S:  8% 85% 7% 8%



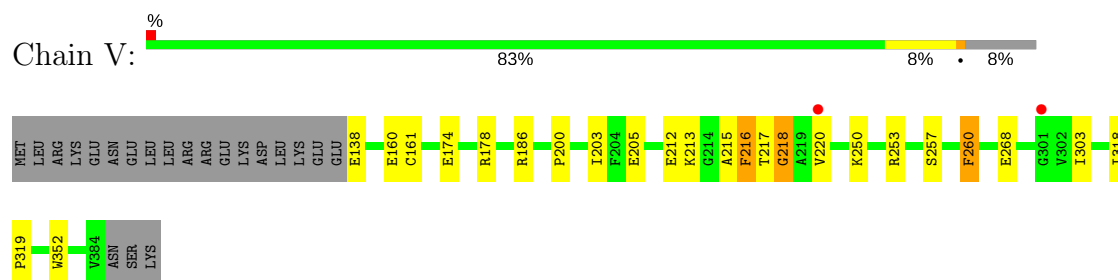
- Molecule 1: Transcriptional regulator (NtrC family)



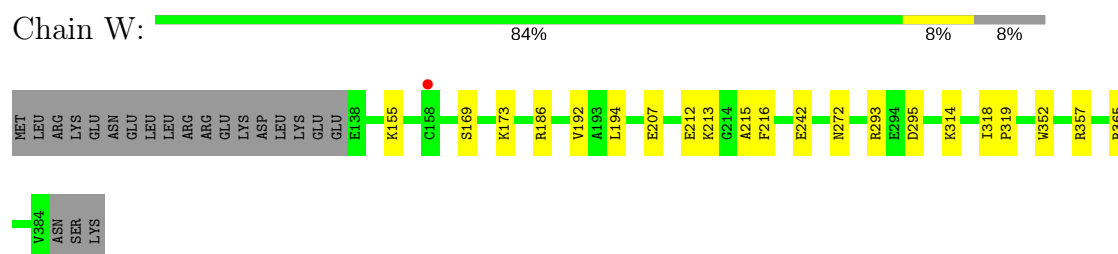
- Molecule 1: Transcriptional regulator (NtrC family)



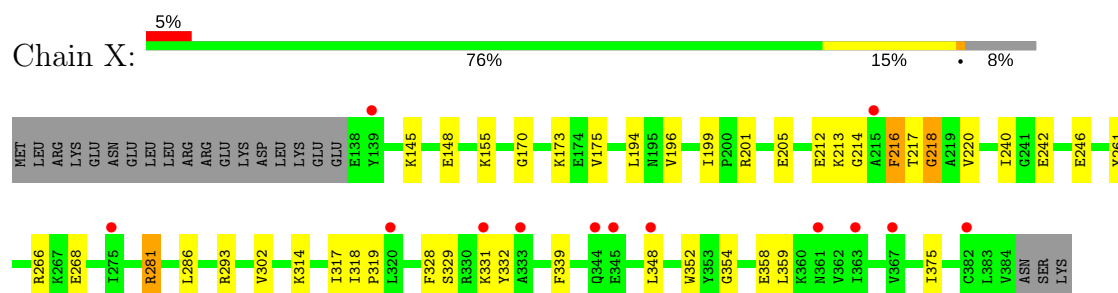
- Molecule 1: Transcriptional regulator (NtrC family)



- Molecule 1: Transcriptional regulator (NtrC family)



- Molecule 1: Transcriptional regulator (NtrC family)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	119.34Å 130.04Å 206.37Å 90.00° 89.73° 89.90°	Depositor
Resolution (Å)	37.85 – 3.60 37.86 – 3.60	Depositor EDS
% Data completeness (in resolution range)	76.2 (37.85-3.60) 69.7 (37.86-3.60)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.66 (at 3.56Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.258 , 0.308 0.253 , 0.301	Depositor DCC
$R_{free}$ test set	5105 reflections (5.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	86.8	Xtriage
Anisotropy	0.943	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 72.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.237 for h,-k,-l 0.319 for -h,k,-l 0.219 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	97439	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	161.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.26% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: MG, ADP, 08T

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	0.24	0/2013	0.45	0/2700
1	B	0.25	0/2013	0.48	0/2700
1	C	0.26	0/2013	0.50	0/2700
1	D	0.27	0/2013	0.50	0/2700
1	E	0.26	0/2013	0.50	0/2700
1	F	0.27	0/2013	0.52	0/2700
1	G	0.24	0/2013	0.46	0/2700
1	H	0.26	0/2013	0.49	0/2700
1	I	0.26	0/2013	0.51	0/2700
1	J	0.27	0/2013	0.49	0/2700
1	K	0.26	0/2013	0.51	0/2700
1	L	0.25	0/2013	0.51	0/2700
1	M	0.25	0/2013	0.48	0/2700
1	N	0.26	0/2013	0.48	0/2700
1	O	0.26	0/2013	0.53	0/2700
1	P	0.27	0/2013	0.52	0/2700
1	Q	0.26	0/2013	0.50	0/2700
1	R	0.27	0/2013	0.65	0/2700
1	S	0.24	0/2013	0.47	0/2700
1	T	0.26	0/2013	0.50	0/2700
1	U	0.26	0/2013	0.51	0/2700
1	V	0.26	0/2013	0.51	0/2700
1	W	0.26	0/2013	0.50	0/2700
1	X	0.28	0/2013	0.62	1/2700 (0.0%)
All	All	0.26	0/48312	0.51	1/64800 (0.0%)

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
1	B	0	1
1	D	0	1
1	F	0	1
1	K	0	1
1	L	0	1
1	N	0	1
1	O	0	1
1	U	0	1
1	V	0	2
1	X	0	1
All	All	0	11

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	218	GLY	N-CA-C	5.07	125.78	113.10

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	215	ALA	Peptide
1	D	216	PHE	Peptide
1	F	215	ALA	Peptide
1	K	214	GLY	Peptide
1	L	216	PHE	Peptide

## 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	1979	2041	2039	15	0
1	B	1979	2042	2040	11	0
1	C	1979	2042	2040	13	0
1	D	1979	2042	2040	22	0
1	E	1979	2042	2040	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1979	2042	2040	23	0
1	G	1979	2042	2040	14	0
1	H	1979	2042	2040	13	0
1	I	1979	2041	2039	17	0
1	J	1979	2042	2040	21	0
1	K	1979	2042	2040	17	0
1	L	1979	2042	2040	18	0
1	M	1979	2042	2040	16	0
1	N	1979	2042	2040	9	0
1	O	1979	2042	2040	27	0
1	P	1979	2042	2040	26	0
1	Q	1979	2042	2040	16	0
1	R	1979	2042	2040	22	0
1	S	1979	2042	2040	14	0
1	T	1979	2041	2039	17	0
1	U	1979	2042	2040	14	0
1	V	1979	2042	2040	16	0
1	W	1979	2042	2040	11	0
1	X	1979	2042	2040	30	0
2	A	31	11	13	2	0
2	B	31	11	13	1	0
2	C	31	11	13	0	0
2	D	31	11	13	3	0
2	E	31	11	13	3	0
2	G	31	11	13	4	0
2	H	31	11	13	1	0
2	I	31	11	13	0	0
2	J	31	11	13	2	0
2	K	31	11	13	1	0
2	M	31	11	13	2	0
2	N	31	11	13	2	0
2	O	31	11	13	7	0
2	P	31	11	13	1	0
2	Q	31	11	13	0	0
2	S	31	11	13	2	0
2	T	31	11	13	1	0
2	U	31	11	13	0	0
2	V	31	11	13	0	0
2	W	31	11	13	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	1	0	0	0	0
3	E	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
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
3	O	1	0	0	0	0
3	P	1	0	0	0	0
3	Q	1	0	0	0	0
3	S	1	0	0	0	0
3	T	1	0	0	0	0
3	U	1	0	0	0	0
3	V	1	0	0	0	0
3	W	1	0	0	0	0
4	L	27	12	12	3	0
4	X	27	12	12	3	0
All	All	48190	49249	49241	383	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 4.

The worst 5 of 383 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:205:GLU:OE1	1:B:250:LYS:NZ	2.11	0.84
1:K:242:GLU:OE2	1:L:293:ARG:NH2	2.13	0.81
1:V:205:GLU:OE1	1:V:250:LYS:NZ	2.12	0.81
1:A:242:GLU:OE2	1:B:293:ARG:NH1	2.14	0.81
1:C:205:GLU:OE2	1:C:250:LYS:NZ	2.13	0.81

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	245/268 (91%)	232 (95%)	12 (5%)	1 (0%)	38	77
1	B	245/268 (91%)	231 (94%)	13 (5%)	1 (0%)	38	77
1	C	245/268 (91%)	230 (94%)	14 (6%)	1 (0%)	38	77
1	D	245/268 (91%)	228 (93%)	14 (6%)	3 (1%)	15	59
1	E	245/268 (91%)	230 (94%)	13 (5%)	2 (1%)	22	65
1	F	245/268 (91%)	221 (90%)	20 (8%)	4 (2%)	11	53
1	G	245/268 (91%)	230 (94%)	14 (6%)	1 (0%)	38	77
1	H	245/268 (91%)	230 (94%)	13 (5%)	2 (1%)	22	65
1	I	245/268 (91%)	233 (95%)	11 (4%)	1 (0%)	38	77
1	J	245/268 (91%)	230 (94%)	12 (5%)	3 (1%)	15	59
1	K	245/268 (91%)	227 (93%)	15 (6%)	3 (1%)	15	59
1	L	245/268 (91%)	226 (92%)	17 (7%)	2 (1%)	22	65
1	M	245/268 (91%)	229 (94%)	15 (6%)	1 (0%)	38	77
1	N	245/268 (91%)	231 (94%)	12 (5%)	2 (1%)	22	65
1	O	245/268 (91%)	230 (94%)	14 (6%)	1 (0%)	38	77
1	P	245/268 (91%)	230 (94%)	13 (5%)	2 (1%)	22	65
1	Q	245/268 (91%)	228 (93%)	14 (6%)	3 (1%)	15	59
1	R	245/268 (91%)	235 (96%)	6 (2%)	4 (2%)	11	53
1	S	245/268 (91%)	232 (95%)	12 (5%)	1 (0%)	38	77
1	T	245/268 (91%)	229 (94%)	14 (6%)	2 (1%)	22	65
1	U	245/268 (91%)	230 (94%)	14 (6%)	1 (0%)	38	77
1	V	245/268 (91%)	228 (93%)	14 (6%)	3 (1%)	15	59
1	W	245/268 (91%)	229 (94%)	13 (5%)	3 (1%)	15	59
1	X	245/268 (91%)	234 (96%)	8 (3%)	3 (1%)	15	59
All	All	5880/6432 (91%)	5513 (94%)	317 (5%)	50 (1%)	20	64

5 of 50 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	196	VAL
1	H	196	VAL
1	J	216	PHE
1	N	196	VAL
1	P	216	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	212/233 (91%)	212 (100%)	0	100	100
1	B	212/233 (91%)	211 (100%)	1 (0%)	91	97
1	C	212/233 (91%)	211 (100%)	1 (0%)	91	97
1	D	212/233 (91%)	209 (99%)	3 (1%)	71	89
1	E	212/233 (91%)	209 (99%)	3 (1%)	71	89
1	F	212/233 (91%)	210 (99%)	2 (1%)	82	92
1	G	212/233 (91%)	212 (100%)	0	100	100
1	H	212/233 (91%)	211 (100%)	1 (0%)	91	97
1	I	212/233 (91%)	212 (100%)	0	100	100
1	J	212/233 (91%)	212 (100%)	0	100	100
1	K	212/233 (91%)	211 (100%)	1 (0%)	91	97
1	L	212/233 (91%)	211 (100%)	1 (0%)	91	97
1	M	212/233 (91%)	211 (100%)	1 (0%)	91	97
1	N	212/233 (91%)	211 (100%)	1 (0%)	91	97
1	O	212/233 (91%)	211 (100%)	1 (0%)	91	97
1	P	212/233 (91%)	209 (99%)	3 (1%)	71	89
1	Q	212/233 (91%)	211 (100%)	1 (0%)	91	97
1	R	212/233 (91%)	208 (98%)	4 (2%)	62	86
1	S	212/233 (91%)	211 (100%)	1 (0%)	91	97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	T	212/233 (91%)	211 (100%)	1 (0%)	91	97
1	U	212/233 (91%)	210 (99%)	2 (1%)	82	92
1	V	212/233 (91%)	211 (100%)	1 (0%)	91	97
1	W	212/233 (91%)	211 (100%)	1 (0%)	91	97
1	X	212/233 (91%)	210 (99%)	2 (1%)	82	92
All	All	5088/5592 (91%)	5056 (99%)	32 (1%)	89	96

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	260	PHE
1	P	217	THR
1	W	216	PHE
1	P	216	PHE
1	P	281	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 42 ligands modelled in this entry, 20 are monoatomic - leaving 22 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link

column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	08T	A	400	1,3	26,33,33	3.24	10 (38%)	24,52,52	2.69	3 (12%)
2	08T	B	400	3	26,33,33	3.23	10 (38%)	24,52,52	2.73	3 (12%)
2	08T	C	400	3	26,33,33	3.21	10 (38%)	24,52,52	2.69	3 (12%)
2	08T	D	400	3	26,33,33	3.23	10 (38%)	24,52,52	2.78	3 (12%)
2	08T	E	400	3	26,33,33	3.22	10 (38%)	24,52,52	2.75	3 (12%)
2	08T	G	400	3	26,33,33	3.26	10 (38%)	24,52,52	2.83	4 (16%)
2	08T	H	400	1,3	26,33,33	3.26	10 (38%)	24,52,52	2.73	6 (25%)
2	08T	I	400	1,3	26,33,33	3.21	10 (38%)	24,52,52	2.70	3 (12%)
2	08T	J	400	3	26,33,33	3.21	10 (38%)	24,52,52	2.80	4 (16%)
2	08T	K	400	-	26,33,33	3.20	10 (38%)	24,52,52	2.69	4 (16%)
4	ADP	L	400	-	25,29,29	0.98	1 (4%)	24,45,45	1.77	2 (8%)
2	08T	M	400	3	26,33,33	3.21	10 (38%)	24,52,52	2.70	3 (12%)
2	08T	N	400	1,3	26,33,33	3.22	10 (38%)	24,52,52	2.82	5 (20%)
2	08T	O	400	3	26,33,33	3.25	9 (34%)	24,52,52	2.67	3 (12%)
2	08T	P	400	3	26,33,33	3.25	10 (38%)	24,52,52	2.70	3 (12%)
2	08T	Q	400	-	26,33,33	3.21	10 (38%)	24,52,52	2.68	4 (16%)
2	08T	S	400	3	26,33,33	3.23	10 (38%)	24,52,52	2.73	3 (12%)
2	08T	T	400	1,3	26,33,33	3.22	10 (38%)	24,52,52	2.69	4 (16%)
2	08T	U	400	1,3	26,33,33	3.23	10 (38%)	24,52,52	2.69	4 (16%)
2	08T	V	400	3	26,33,33	3.22	10 (38%)	24,52,52	2.67	4 (16%)
2	08T	W	400	3	26,33,33	3.21	10 (38%)	24,52,52	2.71	4 (16%)
4	ADP	X	400	-	25,29,29	0.97	1 (4%)	24,45,45	1.76	2 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	08T	A	400	1,3	-	0/12/38/38	0/3/3/3
2	08T	B	400	3	-	0/12/38/38	0/3/3/3
2	08T	C	400	3	-	0/12/38/38	0/3/3/3
2	08T	D	400	3	-	0/12/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	08T	E	400	3	-	0/12/38/38	0/3/3/3
2	08T	G	400	3	-	0/12/38/38	0/3/3/3
2	08T	H	400	1,3	-	0/12/38/38	0/3/3/3
2	08T	I	400	1,3	-	0/12/38/38	0/3/3/3
2	08T	J	400	3	-	0/12/38/38	0/3/3/3
2	08T	K	400	-	-	0/12/38/38	0/3/3/3
4	ADP	L	400	-	-	0/12/32/32	0/3/3/3
2	08T	M	400	3	-	0/12/38/38	0/3/3/3
2	08T	N	400	1,3	-	0/12/38/38	0/3/3/3
2	08T	O	400	3	-	0/12/38/38	0/3/3/3
2	08T	P	400	3	-	0/12/38/38	0/3/3/3
2	08T	Q	400	-	-	0/12/38/38	0/3/3/3
2	08T	S	400	3	-	0/12/38/38	0/3/3/3
2	08T	T	400	1,3	-	0/12/38/38	0/3/3/3
2	08T	U	400	1,3	-	0/12/38/38	0/3/3/3
2	08T	V	400	3	-	0/12/38/38	0/3/3/3
2	08T	W	400	3	-	0/12/38/38	0/3/3/3
4	ADP	X	400	-	-	0/12/32/32	0/3/3/3

The worst 5 of 201 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	400	08T	F2-BE	-7.69	1.34	1.54
2	O	400	08T	F2-BE	-7.54	1.34	1.54
2	H	400	08T	F2-BE	-7.47	1.35	1.54
2	D	400	08T	F2-BE	-7.33	1.35	1.54
2	N	400	08T	F2-BE	-7.31	1.35	1.54

The worst 5 of 77 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	400	08T	N3-C2-N1	-10.24	119.94	128.86
2	D	400	08T	N3-C2-N1	-10.23	119.95	128.86
2	A	400	08T	N3-C2-N1	-10.23	119.95	128.86
2	G	400	08T	N3-C2-N1	-10.21	119.96	128.86
2	H	400	08T	N3-C2-N1	-10.16	120.01	128.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

17 monomers are involved in 39 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	400	08T	2	0
2	B	400	08T	1	0
2	D	400	08T	3	0
2	E	400	08T	3	0
2	G	400	08T	4	0
2	H	400	08T	1	0
2	J	400	08T	2	0
2	K	400	08T	1	0
4	L	400	ADP	3	0
2	M	400	08T	2	0
2	N	400	08T	2	0
2	O	400	08T	7	0
2	P	400	08T	1	0
2	S	400	08T	2	0
2	T	400	08T	1	0
2	W	400	08T	1	0
4	X	400	ADP	3	0

## 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, 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	247/268 (92%)	-0.13	2 (0%) 86 75	141, 179, 214, 236	0
1	B	247/268 (92%)	-0.03	4 (1%) 72 59	87, 146, 181, 196	0
1	C	247/268 (92%)	-0.08	2 (0%) 86 75	90, 138, 183, 202	0
1	D	247/268 (92%)	-0.11	0 100 100	78, 122, 152, 179	0
1	E	247/268 (92%)	-0.04	0 100 100	80, 123, 154, 195	0
1	F	247/268 (92%)	-0.10	3 (1%) 79 66	91, 154, 216, 241	0
1	G	247/268 (92%)	0.31	23 (9%) 9 7	156, 188, 226, 240	0
1	H	247/268 (92%)	-0.08	0 100 100	89, 144, 180, 196	0
1	I	247/268 (92%)	-0.07	1 (0%) 92 87	92, 129, 184, 211	0
1	J	247/268 (92%)	-0.02	2 (0%) 86 75	88, 128, 160, 180	0
1	K	247/268 (92%)	0.02	0 100 100	87, 125, 159, 189	0
1	L	247/268 (92%)	0.16	15 (6%) 22 16	95, 165, 254, 273	0
1	M	247/268 (92%)	-0.03	4 (1%) 72 59	128, 173, 203, 219	0
1	N	247/268 (92%)	-0.05	2 (0%) 86 75	87, 141, 177, 209	0
1	O	247/268 (92%)	-0.10	0 100 100	89, 134, 184, 220	0
1	P	247/268 (92%)	-0.06	0 100 100	83, 126, 157, 186	0
1	Q	247/268 (92%)	-0.00	1 (0%) 92 87	74, 124, 154, 195	0
1	R	247/268 (92%)	-0.01	5 (2%) 65 51	97, 161, 224, 242	0
1	S	247/268 (92%)	0.28	21 (8%) 11 9	155, 190, 226, 239	0
1	T	247/268 (92%)	-0.08	0 100 100	95, 146, 181, 199	0
1	U	247/268 (92%)	-0.06	1 (0%) 92 87	86, 135, 187, 210	0
1	V	247/268 (92%)	-0.08	2 (0%) 86 75	82, 126, 158, 200	0
1	W	247/268 (92%)	-0.10	1 (0%) 92 87	83, 125, 161, 192	0
1	X	247/268 (92%)	0.16	13 (5%) 27 20	102, 165, 252, 273	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
All	All	5928/6432 (92%)	-0.01	102 (1%)	70	57	74, 143, 210, 273	0

The worst 5 of 102 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	363	ILE	7.6
1	X	363	ILE	7.3
1	L	344	GLN	7.0
1	X	344	GLN	6.9
1	G	215	ALA	5.6

## 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 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	08T	K	400	31/31	0.93	0.29	0.26	83,110,130,143	42
2	08T	H	400	31/31	0.89	0.30	0.19	77,111,128,146	42
2	08T	B	400	31/31	0.93	0.29	0.15	79,125,156,158	42
2	08T	N	400	31/31	0.91	0.28	0.08	95,118,141,155	42
3	MG	T	401	1/1	0.95	0.24	0.03	129,129,129,129	0
2	08T	P	400	31/31	0.94	0.29	0.02	80,102,124,131	42
3	MG	C	401	1/1	0.96	0.27	0.02	82,82,82,82	0
2	08T	E	400	31/31	0.92	0.27	-0.00	86,115,137,160	42
3	MG	V	401	1/1	0.92	0.27	0.00	113,113,113,113	0
3	MG	I	401	1/1	0.84	0.27	-0.03	109,109,109,109	0
2	08T	W	400	31/31	0.92	0.26	-0.03	72,105,127,133	42

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	08T	I	400	31/31	0.90	0.28	-0.04	75,109,129,136	42
2	08T	O	400	31/31	0.90	0.27	-0.04	72,118,139,159	42
2	08T	T	400	31/31	0.91	0.27	-0.07	97,122,150,150	42
2	08T	J	400	31/31	0.91	0.28	-0.11	93,118,134,159	42
2	08T	D	400	31/31	0.93	0.26	-0.13	54,97,124,136	42
3	MG	U	401	1/1	0.96	0.20	-0.13	125,125,125,125	0
2	08T	C	400	31/31	0.93	0.27	-0.14	97,123,139,149	42
3	MG	J	401	1/1	0.97	0.25	-0.15	85,85,85,85	0
2	08T	Q	400	31/31	0.92	0.27	-0.20	64,105,127,134	0
2	08T	S	400	31/31	0.89	0.22	-0.35	127,163,203,237	42
2	08T	U	400	31/31	0.93	0.24	-0.38	85,112,140,153	42
2	08T	A	400	31/31	0.89	0.22	-0.39	124,147,166,181	42
2	08T	V	400	31/31	0.93	0.24	-0.39	84,112,126,143	42
2	08T	G	400	31/31	0.89	0.24	-0.53	117,149,177,182	42
3	MG	A	401	1/1	0.97	0.18	-0.54	140,140,140,140	1
4	ADP	X	400	27/27	0.85	0.20	-0.67	153,178,207,214	0
2	08T	M	400	31/31	0.92	0.20	-0.69	129,155,180,188	42
4	ADP	L	400	27/27	0.87	0.21	-0.70	148,178,213,214	39
3	MG	S	401	1/1	0.95	0.14	-1.19	153,153,153,153	0
3	MG	K	401	1/1	0.96	0.19	-1.27	118,118,118,118	1
3	MG	M	401	1/1	0.97	0.15	-1.30	133,133,133,133	1
3	MG	P	401	1/1	0.75	0.21	-1.51	113,113,113,113	0
3	MG	Q	401	1/1	0.66	0.22	-1.80	125,125,125,125	1
3	MG	B	401	1/1	0.88	0.16	-1.82	112,112,112,112	0
3	MG	N	401	1/1	0.88	0.14	-2.00	96,96,96,96	1
3	MG	E	401	1/1	0.89	0.16	-2.49	95,95,95,95	0
3	MG	W	401	1/1	0.92	0.13	-2.91	109,109,109,109	0
3	MG	D	401	1/1	0.90	0.12	-2.94	105,105,105,105	0
3	MG	O	401	1/1	0.86	0.14	-3.39	110,110,110,110	0
3	MG	H	401	1/1	0.81	0.12	-3.77	111,111,111,111	1
3	MG	G	401	1/1	0.72	0.32	-	155,155,155,155	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.