



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 06:39 PM GMT

PDB ID : 4LZZ  
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 : 2013-08-01  
Resolution : 3.21 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

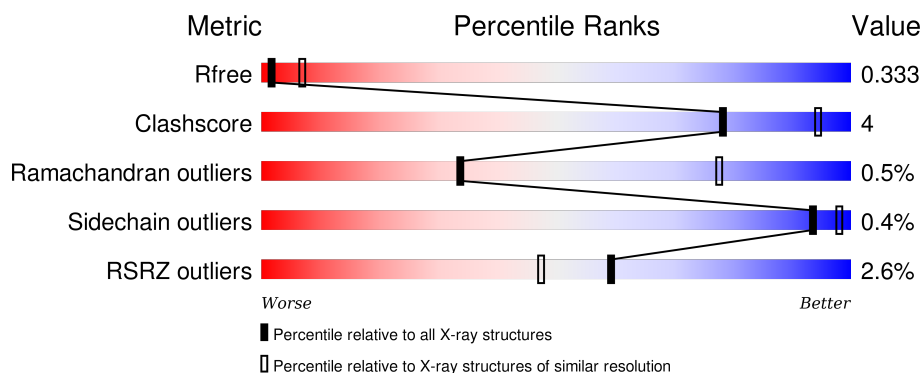
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.21 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))
$R_{free}$	91344	1095 (3.26-3.18)
Clashscore	102246	1046 (3.24-3.20)
Ramachandran outliers	100387	1026 (3.24-3.20)
Sidechain outliers	100360	1025 (3.24-3.20)
RSRZ outliers	91569	1100 (3.26-3.18)

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>4%</div> <div>84% 9% 8%</div> </div>
1	B	268	<div> <div>%</div> <div>84% 7% 8%</div> </div>
1	C	268	<div> <div>85% 7% 8%</div> </div>
1	D	268	<div> <div>85% 7% 8%</div> </div>
1	E	268	<div> <div>85% 10% .</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	268	
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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MG	K	401	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 97749 atoms, of which 49378 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
			4020	1278	2041	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
			4018	1278	2039	333	364	4			
1	E	258	Total	C	H	N	O	S	0	0	0
			4227	1339	2149	352	383	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
			4020	1278	2041	333	364	4			
1	H	247	Total	C	H	N	O	S	0	0	0
			4020	1278	2041	333	364	4			
1	I	248	Total	C	H	N	O	S	0	0	0
			4036	1283	2048	334	367	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
			4019	1278	2040	333	364	4			
1	L	246	Total	C	H	N	O	S	0	0	0
			4006	1273	2036	332	361	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
			4020	1278	2041	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
			4020	1278	2041	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
			4020	1278	2041	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
			4020	1278	2041	333	364	4			
1	T	247	Total	C	H	N	O	S	0	0	0
			4021	1278	2042	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	250	Total	C	H	N	O	S	0	0	0
			4065	1292	2060	337	372	4			
1	X	246	Total	C	H	N	O	S	0	0	0
			4006	1273	2036	332	361	4			

There are 24 discrepancies between the modelled and reference sequences:

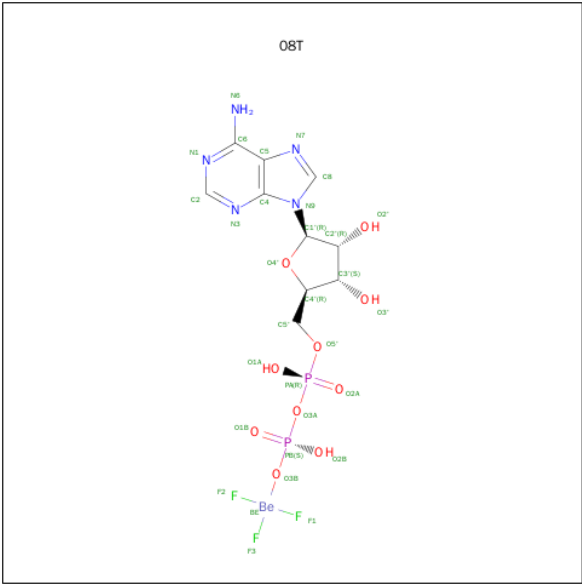
Chain	Residue	Modelled	Actual	Comment	Reference
A	120	MET	-	INITIATING METHIONINE	UNP O67198
B	120	MET	-	INITIATING METHIONINE	UNP O67198
C	120	MET	-	INITIATING METHIONINE	UNP O67198
D	120	MET	-	INITIATING METHIONINE	UNP O67198
E	120	MET	-	INITIATING METHIONINE	UNP O67198
F	120	MET	-	INITIATING METHIONINE	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	R	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		
2	X	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	K	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	W	1	Total	Mg	0	0
			1	1		
3	N	1	Total	Mg	0	0
			1	1		
3	X	1	Total	Mg	0	0
			1	1		

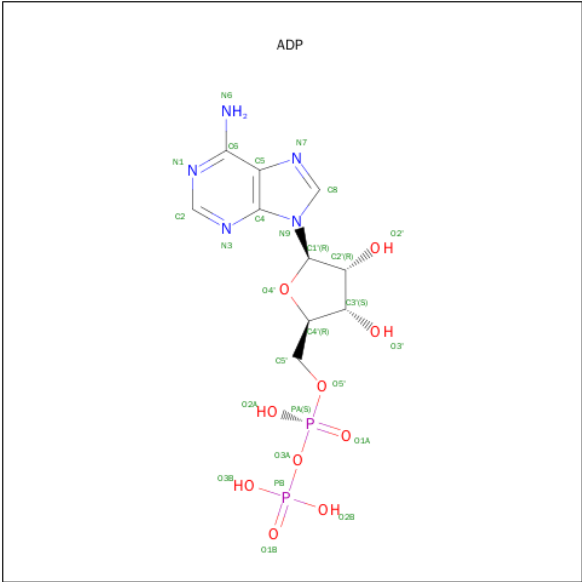
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	S	1	Total 1	Mg 1	0	0
3	J	1	Total 1	Mg 1	0	0
3	E	1	Total 1	Mg 1	0	0
3	V	1	Total 1	Mg 1	0	0
3	A	1	Total 1	Mg 1	0	0
3	R	1	Total 1	Mg 1	0	0
3	D	1	Total 1	Mg 1	0	0
3	I	1	Total 1	Mg 1	0	0
3	U	1	Total 1	Mg 1	0	0
3	L	1	Total 1	Mg 1	0	0
3	G	1	Total 1	Mg 1	0	0
3	Q	1	Total 1	Mg 1	0	0
3	H	1	Total 1	Mg 1	0	0
3	C	1	Total 1	Mg 1	0	0
3	T	1	Total 1	Mg 1	0	0
3	O	1	Total 1	Mg 1	0	0
3	F	1	Total 1	Mg 1	0	0

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



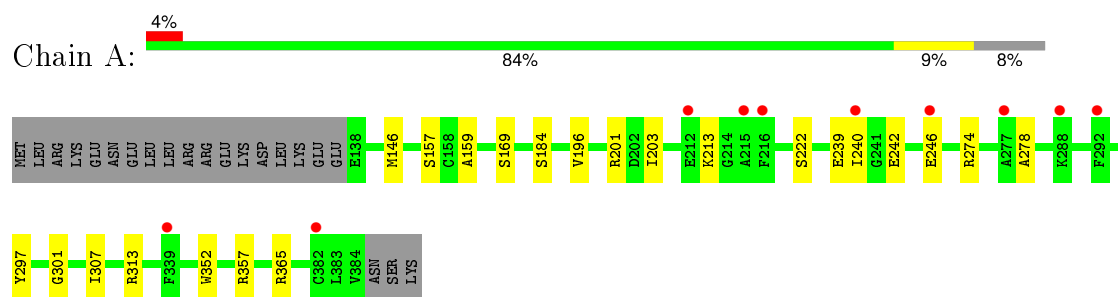


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	F	1	Total	C	H	N	O	P	0	0
			38	10	11	5	10	2		
4	L	1	Total	C	H	N	O	P	0	0
			38	10	11	5	10	2		

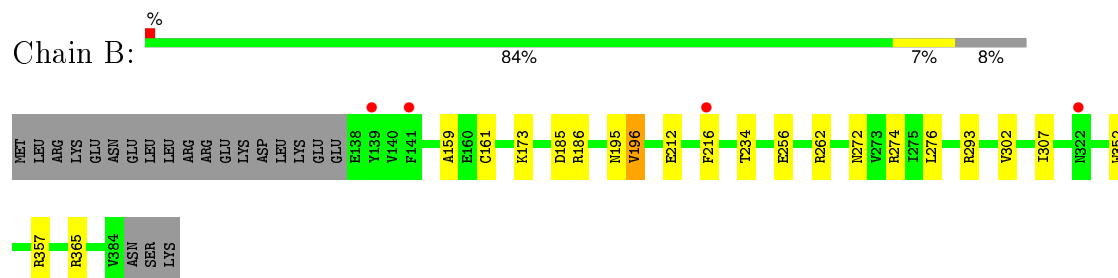
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

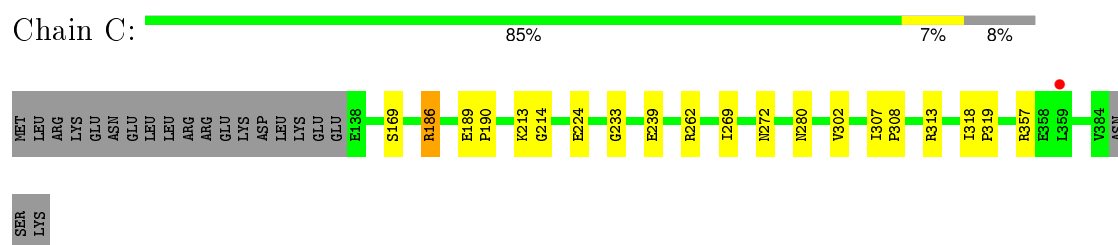
- Molecule 1: Transcriptional regulator (NtrC family)



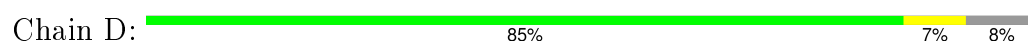
- Molecule 1: Transcriptional regulator (NtrC family)



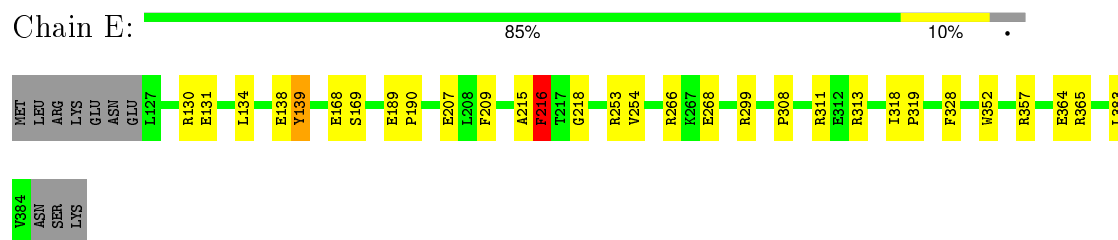
- Molecule 1: Transcriptional regulator (NtrC family)



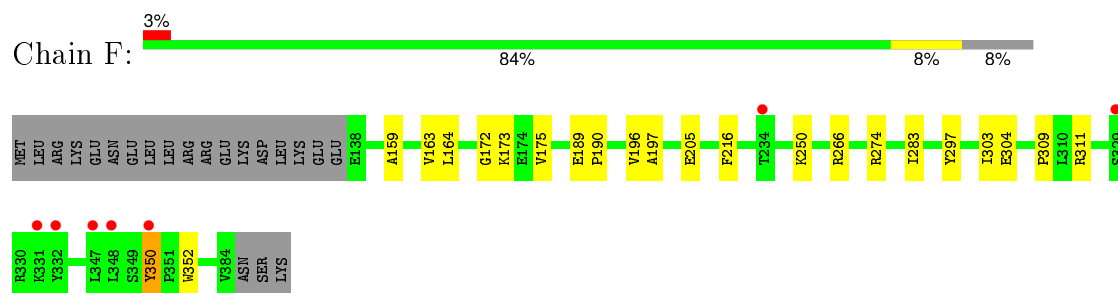
- Molecule 1: Transcriptional regulator (NtrC family)



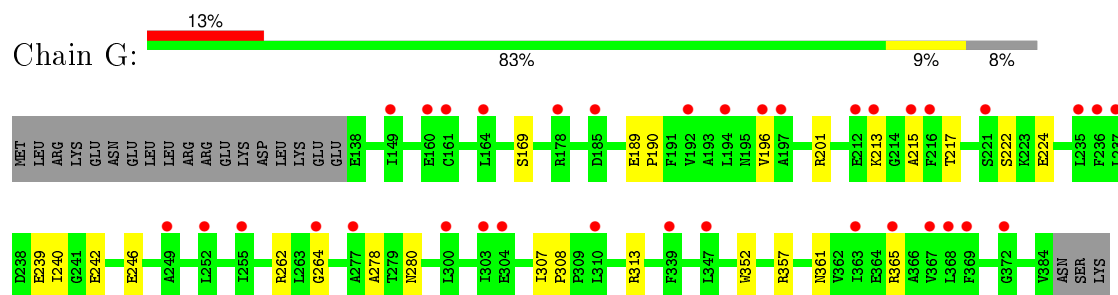
- Molecule 1: Transcriptional regulator (NtrC family)



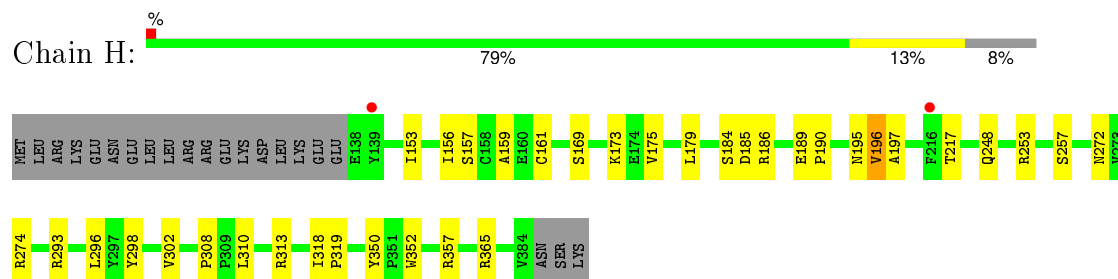
- Molecule 1: Transcriptional regulator (NtrC family)



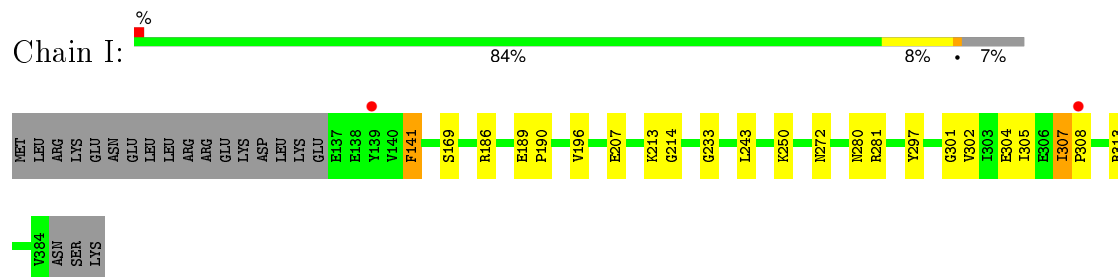
- Molecule 1: Transcriptional regulator (NtrC family)




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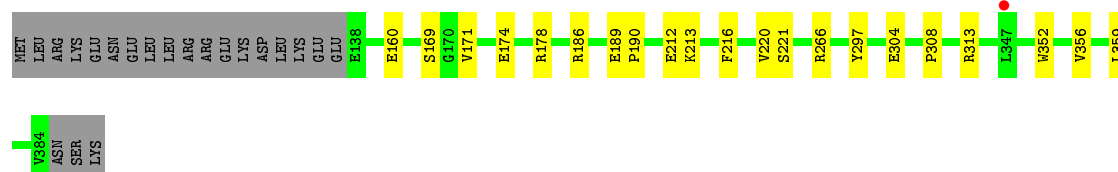
- Molecule 1: Transcriptional regulator (NtrC family)

Chain J: 




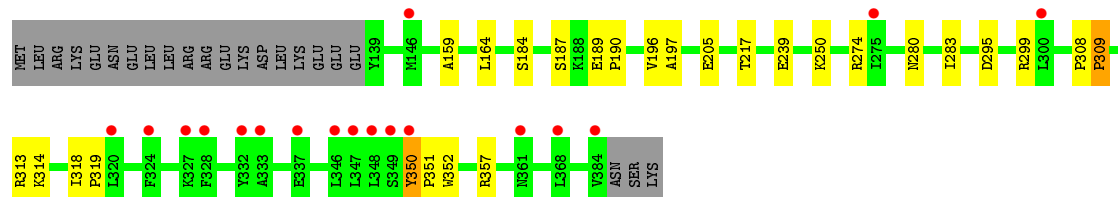
- Molecule 1: Transcriptional regulator (NtrC family)

Chain K: 




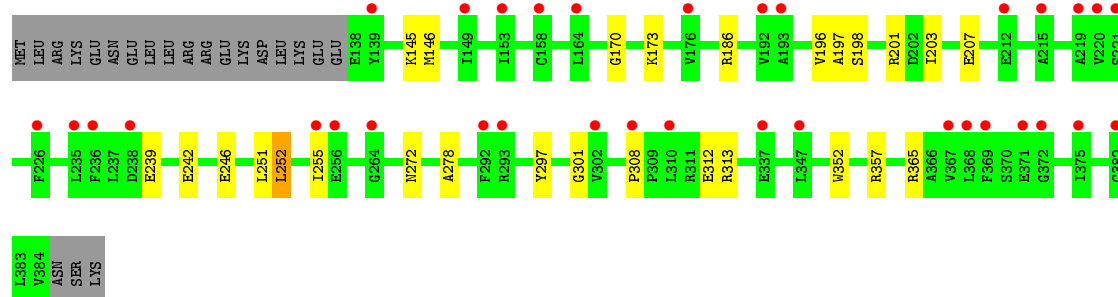
- Molecule 1: Transcriptional regulator (NtrC family)

Chain L: 




- Molecule 1: Transcriptional regulator (NtrC family)

Chain M: 

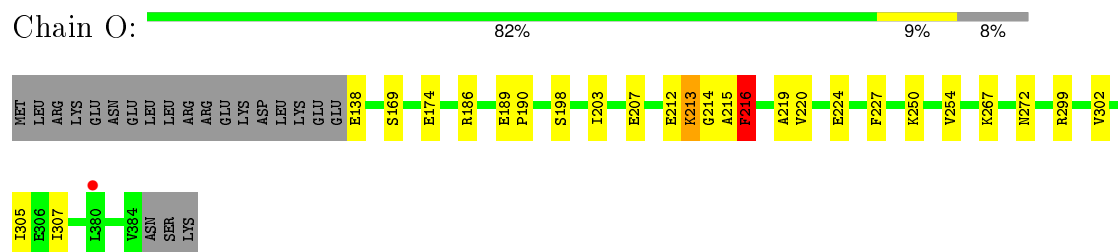


- Molecule 1: Transcriptional regulator (NtrC family)

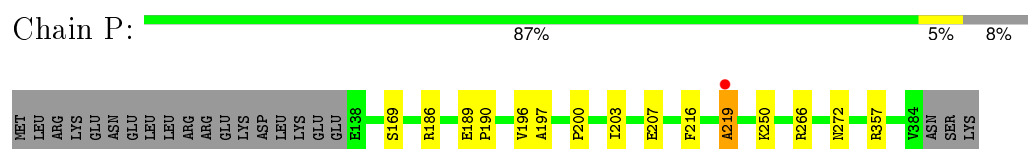
Chain N: 



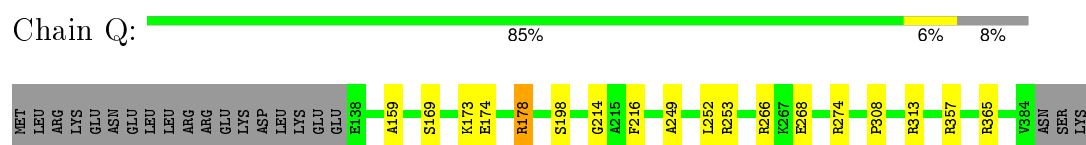
- Molecule 1: Transcriptional regulator (NtrC family)



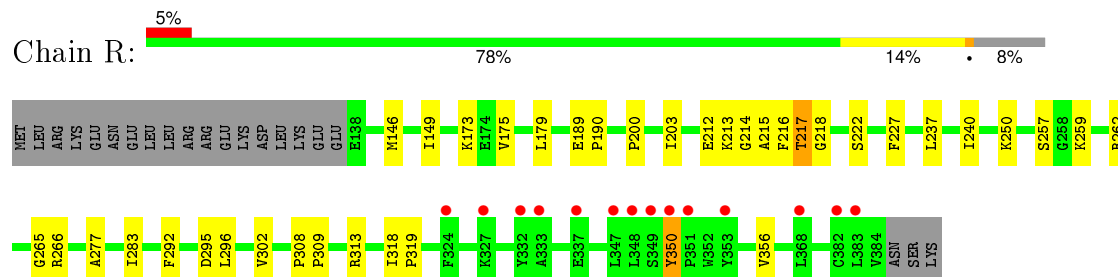
- Molecule 1: Transcriptional regulator (NtrC family)



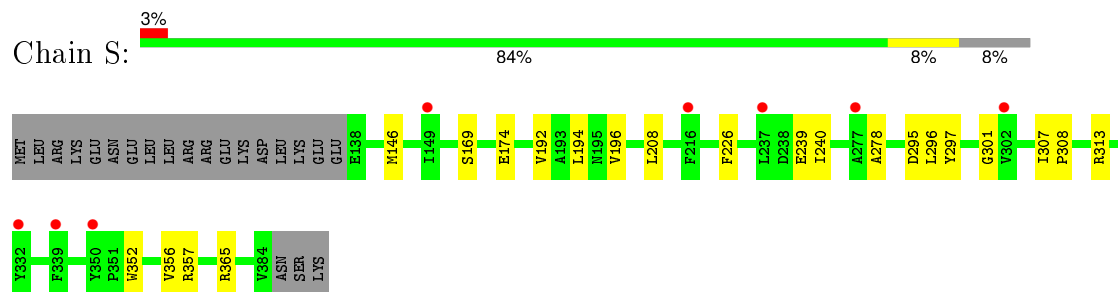
- Molecule 1: Transcriptional regulator (NtrC family)



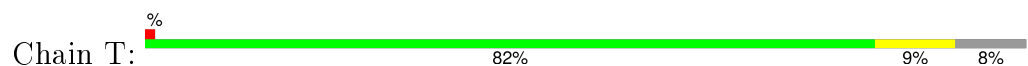
- Molecule 1: Transcriptional regulator (NtrC family)

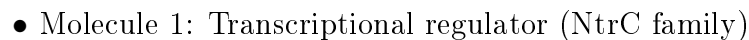


- Molecule 1: Transcriptional regulator (NtrC family)



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- Molecule 1: Transcriptional regulator (NtrC family)

L310	R313	I317	P319	L320	S329	K341	L348	S349	V350	P351	V352	V356	R357	V362	I375	E379	L383	V384	ASN	SRV	LYS
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	119.97Å 130.83Å 208.23Å 90.01° 90.01° 89.85°	Depositor
Resolution (Å)	44.27 – 3.21 44.27 – 3.21	Depositor EDS
% Data completeness (in resolution range)	50.5 (44.27-3.21) 50.5 (44.27-3.21)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.73 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.267 , 0.322 0.278 , 0.333	Depositor DCC
$R_{free}$ test set	1107 reflections (1.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	67.5	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 18.6	EDS
Estimated twinning fraction	0.236 for h,-k,-l 0.359 for -h,k,-l 0.229 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 109010 reflections	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	97749	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.78% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	0.26	0/2013	0.48	0/2700
1	B	0.28	0/2013	0.49	0/2700
1	C	0.28	0/2013	0.49	0/2700
1	D	0.30	0/2013	0.52	0/2700
1	E	0.29	0/2112	0.52	0/2830
1	F	0.28	0/2013	0.54	0/2700
1	G	0.27	0/2013	0.48	0/2700
1	H	0.28	0/2013	0.48	0/2700
1	I	0.29	0/2022	0.51	0/2712
1	J	0.28	0/2013	0.48	0/2700
1	K	0.29	0/2013	0.49	0/2700
1	L	0.27	0/2004	0.52	0/2688
1	M	0.28	0/2013	0.52	0/2700
1	N	0.28	0/2013	0.47	0/2700
1	O	0.30	0/2013	0.55	1/2700 (0.0%)
1	P	0.28	0/2013	0.50	0/2700
1	Q	0.28	0/2013	0.47	0/2700
1	R	0.30	0/2013	0.67	1/2700 (0.0%)
1	S	0.26	0/2013	0.49	0/2700
1	T	0.26	0/2013	0.47	0/2700
1	U	0.28	0/2013	0.49	0/2700
1	V	0.29	0/2013	0.50	0/2700
1	W	0.29	0/2039	0.50	0/2735
1	X	0.30	0/2004	0.65	2/2688 (0.1%)
All	All	0.28	0/48428	0.51	4/64953 (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	D	0	1
1	E	0	1
1	F	0	1
1	L	0	1
1	U	0	2
All	All	0	6

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	349	SER	N-CA-C	-6.83	92.55	111.00
1	R	350	TYR	N-CA-C	5.85	126.79	111.00
1	X	350	TYR	N-CA-C	5.62	126.18	111.00
1	O	216	PHE	CB-CG-CD1	5.19	124.43	120.80

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	216	PHE	Peptide
1	E	216	PHE	Peptide
1	F	350	TYR	Peptide
1	L	350	TYR	Peptide
1	U	213	LYS	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	2041	2039	16	0
1	C	1979	2042	2040	13	0
1	D	1979	2039	2037	13	0
1	E	2078	2149	2147	20	0
1	F	1979	2042	2040	16	0
1	G	1979	2041	2039	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1979	2041	2039	23	0
1	I	1988	2048	2046	15	0
1	J	1979	2042	2040	8	0
1	K	1979	2040	2038	12	0
1	L	1970	2036	2034	14	0
1	M	1979	2042	2040	18	0
1	N	1979	2041	2039	21	0
1	O	1979	2042	2040	21	0
1	P	1979	2041	2039	12	0
1	Q	1979	2041	2039	12	0
1	R	1979	2042	2040	24	0
1	S	1979	2041	2039	14	0
1	T	1979	2042	2040	19	0
1	U	1979	2042	2039	14	0
1	V	1979	2042	2040	16	0
1	W	2005	2060	2058	14	0
1	X	1970	2036	2034	20	0
2	A	31	11	13	1	0
2	B	31	11	13	2	0
2	C	31	11	13	2	0
2	D	31	11	13	5	0
2	E	31	11	13	2	0
2	G	31	11	13	1	0
2	H	31	11	13	2	0
2	I	31	11	13	1	0
2	J	31	11	13	2	0
2	K	31	11	13	3	0
2	M	31	11	13	3	0
2	N	31	11	13	4	0
2	O	31	11	13	2	0
2	P	31	11	13	2	0
2	Q	31	11	12	2	0
2	R	31	11	13	4	0
2	S	31	11	13	3	0
2	T	31	11	13	7	0
2	U	31	11	13	2	0
2	V	31	11	13	3	0
2	W	31	11	13	2	0
2	X	31	11	13	4	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	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
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	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	R	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
3	X	1	0	0	0	0
4	F	27	11	12	3	0
4	L	27	11	12	1	0
All	All	48371	49378	49374	347	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 347 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:M:146:MET:SD	1:M:313:ARG:NH2	2.51	0.83
1:O:219:ALA:HB1	1:O:220:VAL:HA	1.61	0.82
1:T:186:ARG:NH2	1:T:272:ASN:OD1	2.13	0.82
1:B:186:ARG:NH2	1:B:272:ASN:OD1	2.15	0.79
1:M:357:ARG:NH1	2:M:400:08T:O3'	2.17	0.78

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%)	231 (94%)	13 (5%)	1 (0%)	39	80
1	B	245/268 (91%)	234 (96%)	9 (4%)	2 (1%)	24	69
1	C	245/268 (91%)	232 (95%)	12 (5%)	1 (0%)	39	80
1	D	245/268 (91%)	233 (95%)	12 (5%)	0	100	100
1	E	256/268 (96%)	237 (93%)	16 (6%)	3 (1%)	16	60
1	F	245/268 (91%)	234 (96%)	10 (4%)	1 (0%)	39	80
1	G	245/268 (91%)	231 (94%)	13 (5%)	1 (0%)	39	80
1	H	245/268 (91%)	234 (96%)	9 (4%)	2 (1%)	24	69
1	I	246/268 (92%)	234 (95%)	11 (4%)	1 (0%)	39	80
1	J	245/268 (91%)	234 (96%)	11 (4%)	0	100	100
1	K	245/268 (91%)	235 (96%)	10 (4%)	0	100	100
1	L	244/268 (91%)	229 (94%)	12 (5%)	3 (1%)	16	60
1	M	245/268 (91%)	228 (93%)	15 (6%)	2 (1%)	24	69
1	N	245/268 (91%)	234 (96%)	9 (4%)	2 (1%)	24	69
1	O	245/268 (91%)	231 (94%)	13 (5%)	1 (0%)	39	80
1	P	245/268 (91%)	233 (95%)	11 (4%)	1 (0%)	39	80
1	Q	245/268 (91%)	236 (96%)	9 (4%)	0	100	100
1	R	245/268 (91%)	233 (95%)	9 (4%)	3 (1%)	16	60
1	S	245/268 (91%)	232 (95%)	12 (5%)	1 (0%)	39	80
1	T	245/268 (91%)	231 (94%)	12 (5%)	2 (1%)	24	69
1	U	245/268 (91%)	233 (95%)	11 (4%)	1 (0%)	39	80
1	V	245/268 (91%)	235 (96%)	9 (4%)	1 (0%)	39	80
1	W	248/268 (92%)	238 (96%)	9 (4%)	1 (0%)	39	80
1	X	244/268 (91%)	232 (95%)	10 (4%)	2 (1%)	24	69
All	All	5893/6432 (92%)	5594 (95%)	267 (4%)	32 (0%)	34	77

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	196	VAL
1	H	196	VAL
1	N	196	VAL
1	R	217	THR
1	R	350	TYR

### 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%)	212 (100%)	0	100	100
1	C	212/233 (91%)	211 (100%)	1 (0%)	92	97
1	D	212/233 (91%)	212 (100%)	0	100	100
1	E	223/233 (96%)	222 (100%)	1 (0%)	93	98
1	F	212/233 (91%)	211 (100%)	1 (0%)	92	97
1	G	212/233 (91%)	212 (100%)	0	100	100
1	H	212/233 (91%)	211 (100%)	1 (0%)	92	97
1	I	213/233 (91%)	212 (100%)	1 (0%)	92	97
1	J	212/233 (91%)	211 (100%)	1 (0%)	92	97
1	K	212/233 (91%)	211 (100%)	1 (0%)	92	97
1	L	211/233 (91%)	211 (100%)	0	100	100
1	M	212/233 (91%)	212 (100%)	0	100	100
1	N	212/233 (91%)	212 (100%)	0	100	100
1	O	212/233 (91%)	210 (99%)	2 (1%)	84	95
1	P	212/233 (91%)	212 (100%)	0	100	100
1	Q	212/233 (91%)	210 (99%)	2 (1%)	84	95
1	R	212/233 (91%)	211 (100%)	1 (0%)	92	97
1	S	212/233 (91%)	212 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	T	212/233 (91%)	212 (100%)	0	100	100
1	U	212/233 (91%)	211 (100%)	1 (0%)	92	97
1	V	212/233 (91%)	211 (100%)	1 (0%)	92	97
1	W	215/233 (92%)	214 (100%)	1 (0%)	92	97
1	X	211/233 (91%)	208 (99%)	3 (1%)	74	91
All	All	5101/5592 (91%)	5083 (100%)	18 (0%)	93	98

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	267	LYS
1	Q	178	ARG
1	W	216	PHE
1	K	216	PHE
1	O	216	PHE

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 47 ligands modelled in this entry, 23 are monoatomic - leaving 24 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	3.15	9 (34%)	28,52,52	3.04	9 (32%)
2	08T	B	400	1,3	26,33,33	3.21	9 (34%)	28,52,52	3.03	10 (35%)
2	08T	C	400	3	26,33,33	3.17	9 (34%)	28,52,52	3.08	8 (28%)
2	08T	D	400	1,3	26,33,33	3.17	9 (34%)	28,52,52	3.08	9 (32%)
2	08T	E	400	3	26,33,33	3.19	9 (34%)	28,52,52	2.98	8 (28%)
4	ADP	F	400	3	22,29,29	0.92	1 (4%)	27,45,45	2.04	5 (18%)
2	08T	G	400	1,3	26,33,33	3.19	9 (34%)	28,52,52	3.07	11 (39%)
2	08T	H	400	1,3	26,33,33	3.19	9 (34%)	28,52,52	3.06	9 (32%)
2	08T	I	400	3	26,33,33	3.18	9 (34%)	28,52,52	3.00	8 (28%)
2	08T	J	400	3	26,33,33	3.22	9 (34%)	28,52,52	3.07	9 (32%)
2	08T	K	400	1,3	26,33,33	3.16	9 (34%)	28,52,52	3.18	9 (32%)
4	ADP	L	400	-	22,29,29	1.05	2 (9%)	27,45,45	1.97	3 (11%)
2	08T	M	400	1	26,33,33	3.16	9 (34%)	28,52,52	3.00	10 (35%)
2	08T	N	400	1,3	26,33,33	3.22	9 (34%)	28,52,52	3.02	11 (39%)
2	08T	O	400	3	26,33,33	3.18	9 (34%)	28,52,52	3.11	9 (32%)
2	08T	P	400	1,3	26,33,33	3.17	9 (34%)	28,52,52	3.02	10 (35%)
2	08T	Q	400	1	26,33,33	3.13	9 (34%)	28,52,52	3.50	9 (32%)
2	08T	R	400	3	26,33,33	3.17	9 (34%)	28,52,52	3.23	8 (28%)
2	08T	S	400	1,3	26,33,33	3.18	9 (34%)	28,52,52	3.03	9 (32%)
2	08T	T	400	1,3	26,33,33	3.19	9 (34%)	28,52,52	3.00	9 (32%)
2	08T	U	400	1,3	26,33,33	3.17	9 (34%)	28,52,52	3.14	9 (32%)
2	08T	V	400	3	26,33,33	3.16	9 (34%)	28,52,52	3.09	8 (28%)
2	08T	W	400	3	26,33,33	3.21	9 (34%)	28,52,52	3.10	8 (28%)
2	08T	X	400	-	26,33,33	3.13	9 (34%)	28,52,52	3.04	10 (35%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	08T	B	400	1,3	-	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	1,3	-	0/12/38/38	0/3/3/3
2	08T	E	400	3	-	0/12/38/38	0/3/3/3
4	ADP	F	400	3	-	0/12/32/32	0/3/3/3
2	08T	G	400	1,3	-	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	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	1,3	-	0/12/38/38	0/3/3/3
4	ADP	L	400	-	-	0/12/32/32	0/3/3/3
2	08T	M	400	1	-	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	1,3	-	0/12/38/38	0/3/3/3
2	08T	Q	400	1	-	0/12/38/38	0/3/3/3
2	08T	R	400	3	-	0/12/38/38	0/3/3/3
2	08T	S	400	1,3	-	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
2	08T	X	400	-	-	0/12/38/38	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	N	400	08T	F2-BE	-7.44	1.35	1.54
2	C	400	08T	F2-BE	-7.41	1.35	1.54
2	D	400	08T	F2-BE	-7.40	1.35	1.54
2	I	400	08T	F2-BE	-7.35	1.35	1.54
2	J	400	08T	F2-BE	-7.35	1.35	1.54

The worst 5 of 208 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	400	08T	N3-C2-N1	-11.94	119.75	128.89
2	R	400	08T	N3-C2-N1	-11.85	119.82	128.89
2	I	400	08T	N3-C2-N1	-11.81	119.85	128.89
2	S	400	08T	N3-C2-N1	-11.72	119.92	128.89
2	Q	400	08T	N3-C2-N1	-11.68	119.95	128.89



There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

24 monomers are involved in 63 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	400	08T	1	0
2	B	400	08T	2	0
2	C	400	08T	2	0
2	D	400	08T	5	0
2	E	400	08T	2	0
4	F	400	ADP	3	0
2	G	400	08T	1	0
2	H	400	08T	2	0
2	I	400	08T	1	0
2	J	400	08T	2	0
2	K	400	08T	3	0
4	L	400	ADP	1	0
2	M	400	08T	3	0
2	N	400	08T	4	0
2	O	400	08T	2	0
2	P	400	08T	2	0
2	Q	400	08T	2	0
2	R	400	08T	4	0
2	S	400	08T	3	0
2	T	400	08T	7	0
2	U	400	08T	2	0
2	V	400	08T	3	0
2	W	400	08T	2	0
2	X	400	08T	4	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%)	0.32	10 (4%) 42 29	84, 119, 143, 157	0
1	B	247/268 (92%)	0.22	4 (1%) 74 64	44, 88, 117, 132	0
1	C	247/268 (92%)	0.11	1 (0%) 93 90	38, 73, 116, 139	0
1	D	247/268 (92%)	0.10	0 100 100	32, 61, 90, 113	0
1	E	258/268 (96%)	0.18	0 100 100	33, 64, 92, 132	8 (3%)
1	F	247/268 (92%)	0.22	7 (2%) 56 44	41, 83, 142, 177	0
1	G	247/268 (92%)	0.75	35 (14%) 4 3	95, 136, 162, 175	0
1	H	247/268 (92%)	0.18	2 (0%) 87 80	51, 88, 115, 136	0
1	I	248/268 (92%)	0.15	2 (0%) 87 80	33, 76, 110, 127	0
1	J	247/268 (92%)	0.15	0 100 100	42, 70, 96, 105	0
1	K	247/268 (92%)	0.13	1 (0%) 93 90	38, 64, 91, 122	0
1	L	246/268 (91%)	0.45	18 (7%) 18 11	41, 87, 165, 193	0
1	M	247/268 (92%)	0.80	34 (13%) 4 3	101, 134, 159, 181	0
1	N	247/268 (92%)	0.19	2 (0%) 87 80	49, 88, 121, 137	0
1	O	247/268 (92%)	0.15	1 (0%) 93 90	35, 72, 113, 134	0
1	P	247/268 (92%)	0.14	1 (0%) 93 90	40, 69, 98, 121	0
1	Q	247/268 (92%)	0.13	0 100 100	41, 68, 92, 117	0
1	R	247/268 (92%)	0.37	14 (5%) 27 17	48, 91, 164, 182	0
1	S	247/268 (92%)	0.23	8 (3%) 51 38	86, 115, 140, 153	0
1	T	247/268 (92%)	0.18	3 (1%) 81 71	45, 90, 123, 143	0
1	U	247/268 (92%)	0.19	1 (0%) 93 90	39, 77, 116, 135	0
1	V	247/268 (92%)	0.12	0 100 100	36, 62, 95, 121	0
1	W	250/268 (93%)	0.17	0 100 100	33, 63, 95, 116	1 (0%)
1	X	246/268 (91%)	0.26	8 (3%) 50 37	40, 85, 146, 182	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
All	All	5941/6432 (92%)	0.24	152 (2%)	59	47	32, 81, 142, 193	9 (0%)

The worst 5 of 152 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	372	GLY	10.9
1	M	221	SER	10.7
1	X	348	LEU	7.9
1	G	216	PHE	7.1
1	G	149	ILE	6.7

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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
3	MG	K	401	1/1	0.99	0.33	3.03	46,46,46,46	0
2	08T	G	400	31/31	0.86	0.38	1.12	93,105,129,132	42
4	ADP	F	400	27/27	0.83	0.30	0.73	71,91,118,119	38
3	MG	G	401	1/1	0.90	0.26	0.41	98,98,98,98	1
3	MG	E	401	1/1	0.98	0.25	0.38	55,55,55,55	0
2	08T	K	400	31/31	0.97	0.27	0.33	42,59,74,81	42
3	MG	N	401	1/1	0.98	0.26	0.22	62,62,62,62	1
2	08T	O	400	31/31	0.92	0.30	0.22	46,61,78,82	42
2	08T	C	400	31/31	0.95	0.27	0.20	39,63,75,88	42
2	08T	N	400	31/31	0.91	0.28	0.07	51,76,92,99	42
2	08T	E	400	31/31	0.96	0.26	0.05	44,57,69,80	42

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	08T	M	400	31/31	0.92	0.27	0.05	88,102,120,128	42
2	08T	T	400	31/31	0.92	0.27	0.02	45,81,97,100	42
2	08T	U	400	31/31	0.95	0.26	-0.06	48,68,82,83	42
2	08T	H	400	31/31	0.95	0.27	-0.10	62,73,87,90	42
2	08T	A	400	31/31	0.93	0.26	-0.11	77,92,110,125	42
3	MG	U	401	1/1	0.91	0.24	-0.18	70,70,70,70	1
2	08T	S	400	31/31	0.93	0.26	-0.18	72,95,115,119	42
2	08T	Q	400	31/31	0.96	0.24	-0.29	36,65,79,83	0
2	08T	I	400	31/31	0.94	0.28	-0.29	50,63,78,85	42
2	08T	B	400	31/31	0.94	0.26	-0.32	50,70,87,94	42
2	08T	W	400	31/31	0.97	0.24	-0.48	40,55,70,74	42
2	08T	P	400	31/31	0.98	0.23	-0.58	47,59,75,81	0
2	08T	J	400	31/31	0.96	0.23	-0.58	51,64,77,87	0
2	08T	D	400	31/31	0.95	0.23	-0.65	42,63,82,85	0
2	08T	X	400	31/31	0.91	0.21	-0.65	74,98,116,126	0
3	MG	A	401	1/1	0.98	0.17	-0.67	54,54,54,54	0
2	08T	R	400	31/31	0.94	0.20	-0.69	93,110,133,149	0
4	ADP	L	400	27/27	0.94	0.22	-0.69	76,95,114,139	0
3	MG	T	401	1/1	0.97	0.21	-0.71	68,68,68,68	1
2	08T	V	400	31/31	0.98	0.22	-0.76	34,56,71,75	0
3	MG	Q	401	1/1	0.86	0.20	-0.84	57,57,57,57	1
3	MG	W	401	1/1	0.99	0.22	-1.05	51,51,51,51	1
3	MG	I	401	1/1	0.94	0.21	-1.09	61,61,61,61	1
3	MG	S	401	1/1	0.97	0.16	-1.20	64,64,64,64	0
3	MG	B	401	1/1	0.89	0.20	-1.23	62,62,62,62	1
3	MG	P	401	1/1	0.95	0.19	-1.42	56,56,56,56	1
3	MG	C	401	1/1	0.95	0.17	-1.51	51,51,51,51	1
3	MG	R	401	1/1	0.92	0.16	-1.68	100,100,100,100	1
3	MG	F	401	1/1	0.87	0.16	-1.81	79,79,79,79	1
3	MG	V	401	1/1	0.99	0.16	-2.23	53,53,53,53	1
3	MG	D	401	1/1	0.95	0.17	-2.38	57,57,57,57	1
3	MG	H	401	1/1	0.96	0.18	-2.57	51,51,51,51	0
3	MG	O	401	1/1	0.92	0.16	-3.85	71,71,71,71	1
3	MG	J	401	1/1	0.93	0.14	-4.03	57,57,57,57	0
3	MG	L	401	1/1	0.95	0.20	-	63,63,63,63	0
3	MG	X	401	1/1	0.98	0.13	-	77,77,77,77	1

## 6.5 Other polymers

There are no such residues in this entry.