



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:41 PM 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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at 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.

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

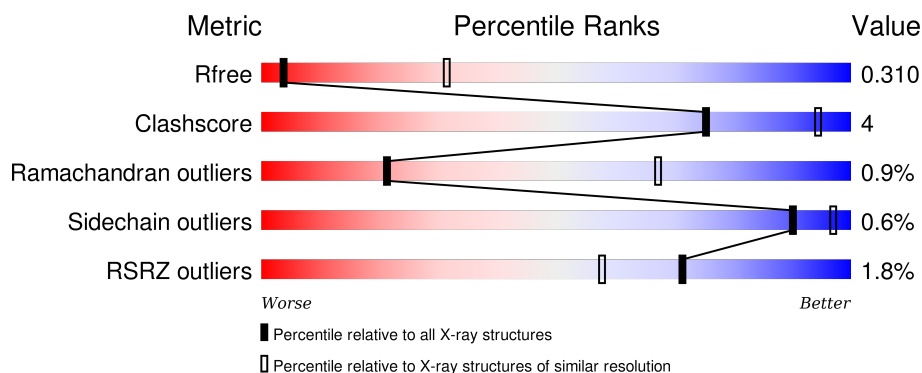
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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}	91344	1408 (3.80-3.40)
Clashscore	102246	1010 (3.74-3.46)
Ramachandran outliers	100387	1007 (3.76-3.44)
Sidechain outliers	100360	1007 (3.76-3.44)
RSRZ outliers	91569	1003 (3.78-3.42)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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>84% 9% 8%</div> </div>
1	B	268	<div> <div></div> <div>85% 7% 8%</div> </div>
1	C	268	<div> <div></div> <div>84% 9% 8%</div> </div>
1	D	268	<div> <div></div> <div>80% 11% 8%</div> </div>
1	E	268	<div> <div></div> <div>83% 9% 8%</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	

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:

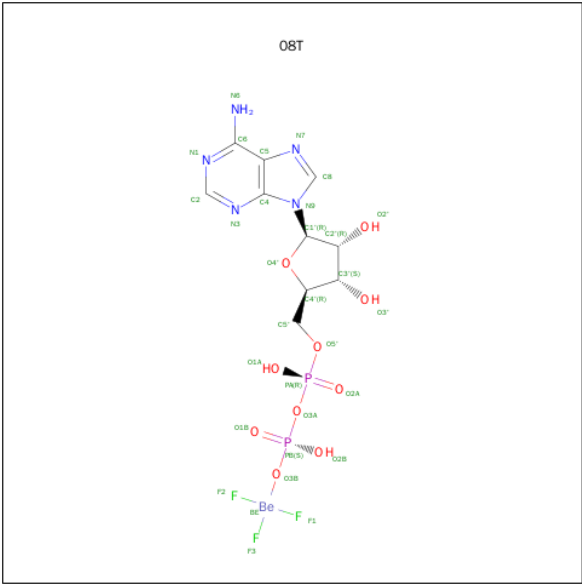
Chain	Residue	Modelled	Actual	Comment	Reference
A	120	MET	-	INITIATING METHIONINE	UNP O67198
B	120	MET	-	INITIATING METHIONINE	UNP O67198
C	120	MET	-	INITIATING METHIONINE	UNP O67198
D	120	MET	-	INITIATING METHIONINE	UNP O67198
E	120	MET	-	INITIATING METHIONINE	UNP O67198
F	120	MET	-	INITIATING METHIONINE	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: C₁₀H₁₄BeF₃N₅O₁₀P₂).



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).

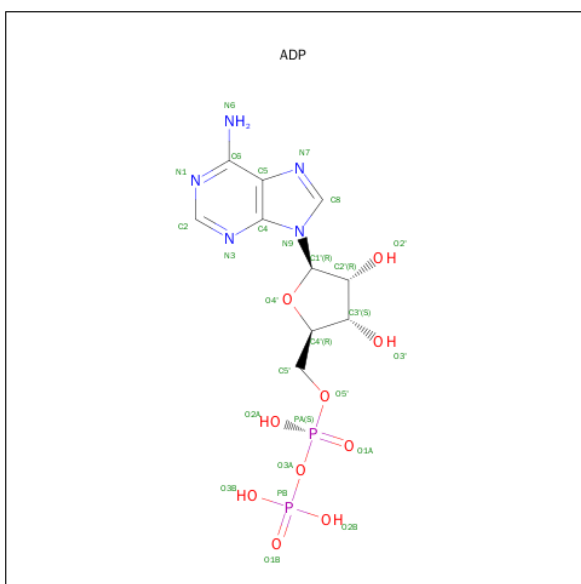
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	P	1	Total	Mg	0	0
			1	1		
3	G	1	Total	Mg	0	0
			1	1		
3	J	1	Total	Mg	0	0
			1	1		
3	Q	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	K	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	H	1	Total	Mg	0	0
			1	1		

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

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

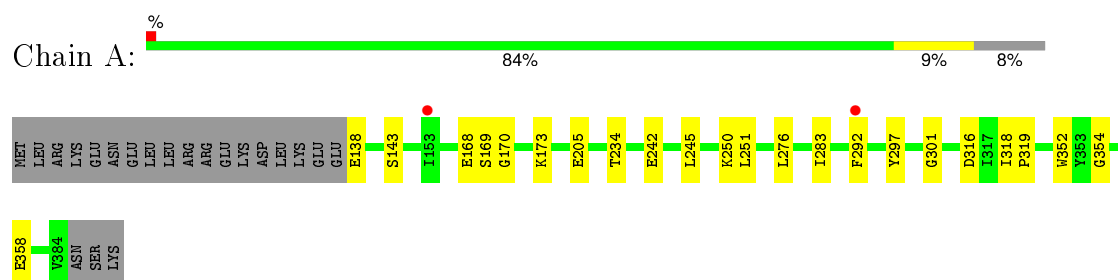


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	L	1	Total	C	H	N	O	P	0	0
			39	10	12	5	10	2		
4	X	1	Total	C	H	N	O	P	0	0
			39	10	12	5	10	2		

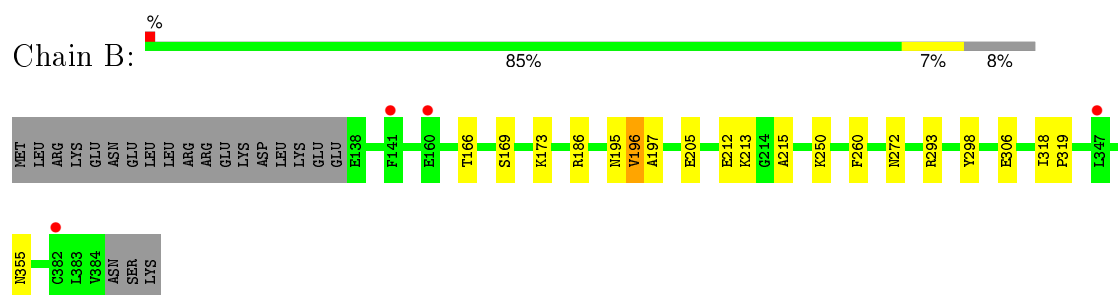
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ($\text{RSRZ} > 2$). 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.

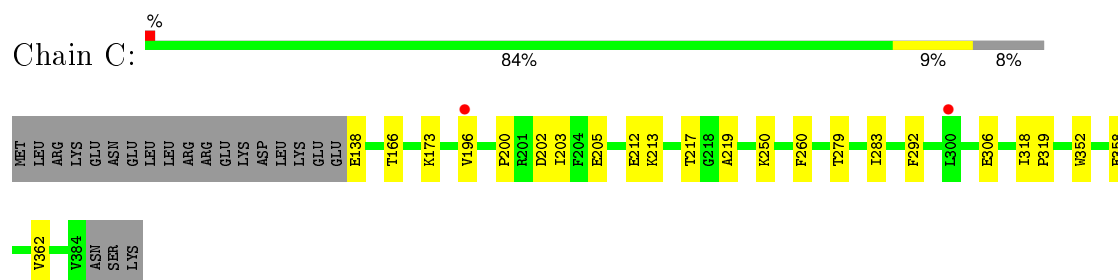
- Molecule 1: Transcriptional regulator (NtrC family)



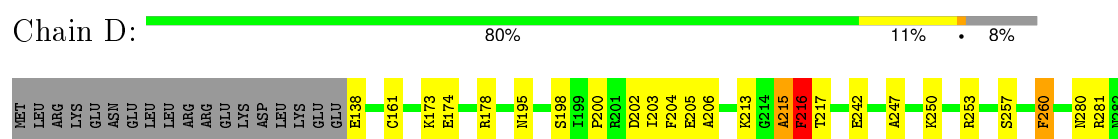
- Molecule 1: Transcriptional regulator (NtrC family)



- Molecule 1: Transcriptional regulator (NtrC family)



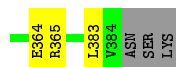
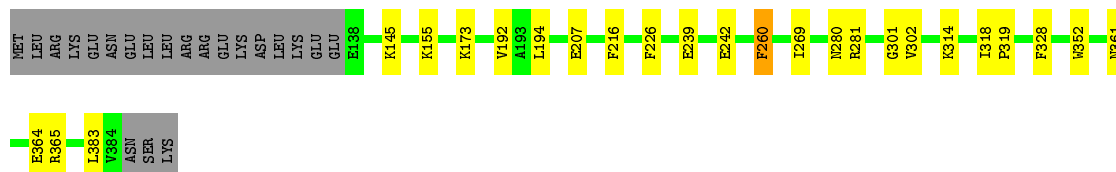
- Molecule 1: Transcriptional regulator (NtrC family)





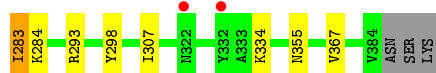
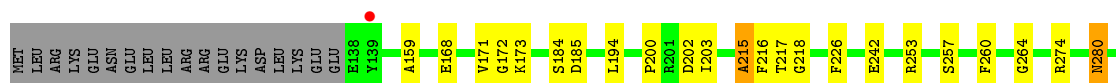
- Molecule 1: Transcriptional regulator (NtrC family)

Chain E: 83% 9% 8%



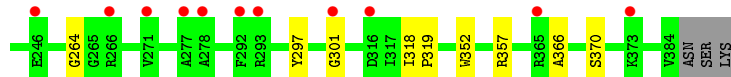
- Molecule 1: Transcriptional regulator (NtrC family)

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%

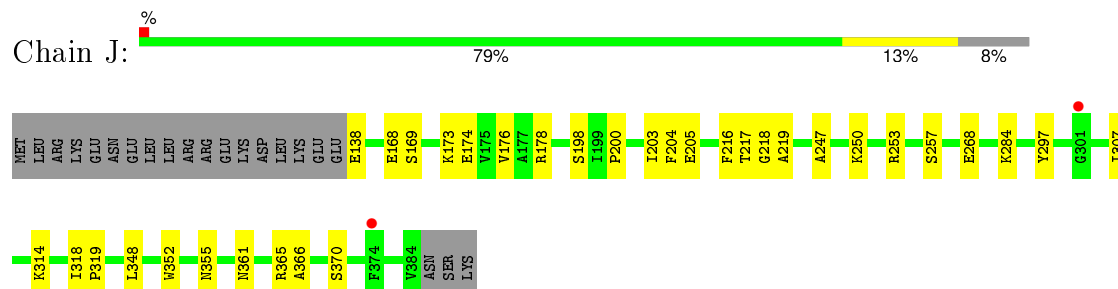


- Molecule 1: Transcriptional regulator (NtrC family)

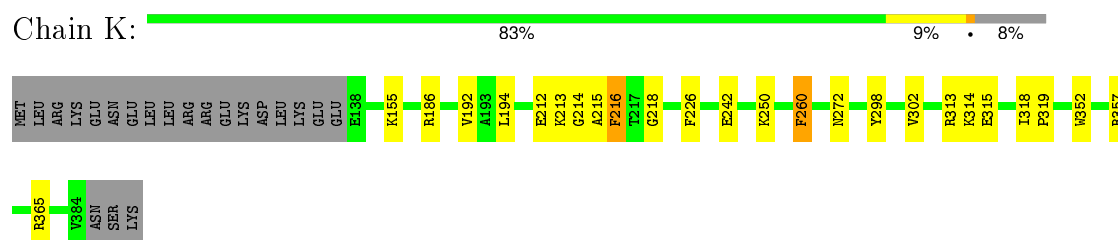
Chain I: 81% 11% 8%



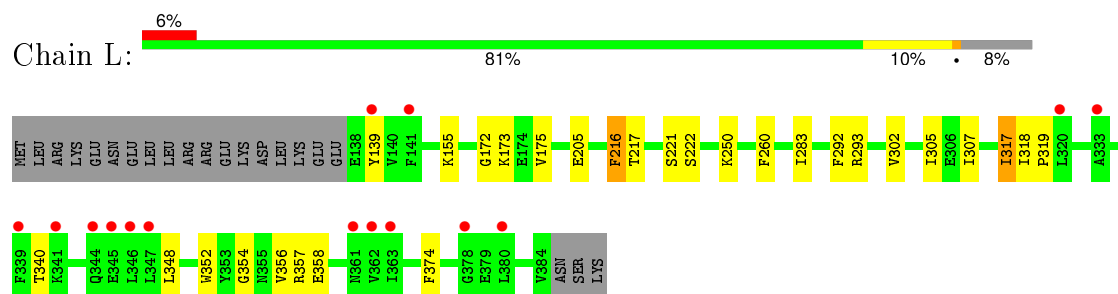
- Molecule 1: Transcriptional regulator (NtrC family)



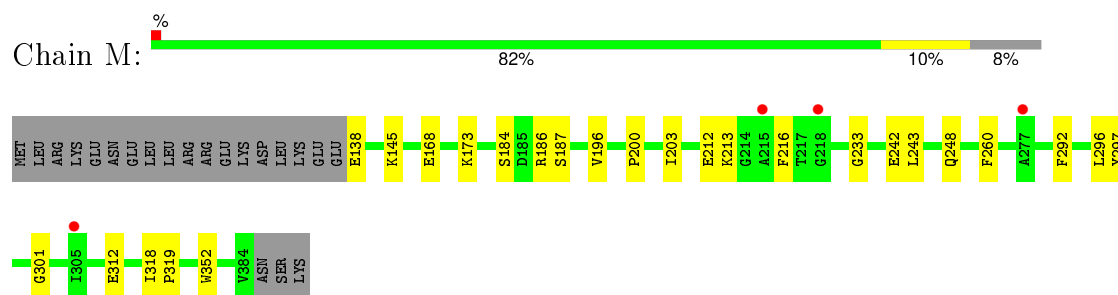
- Molecule 1: Transcriptional regulator (NtrC family)



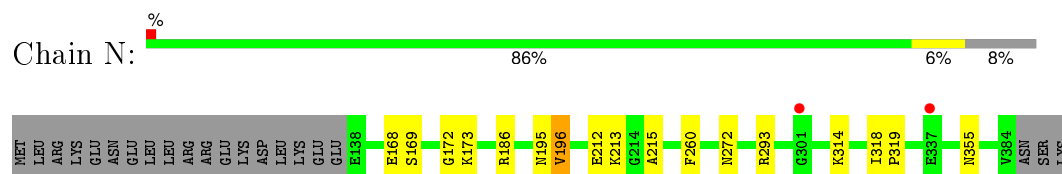
- Molecule 1: Transcriptional regulator (NtrC family)




- Molecule 1: Transcriptional regulator (NtrC family)

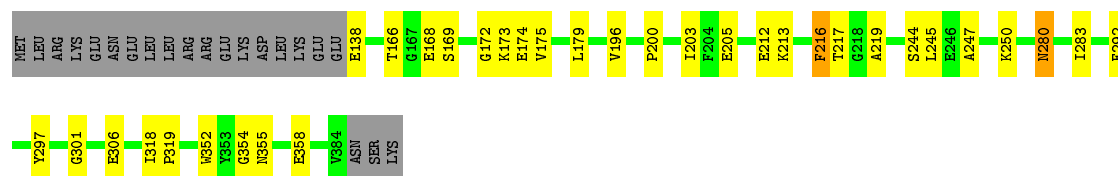


- Molecule 1: Transcriptional regulator (NtrC family)




- Molecule 1: Transcriptional regulator (NtrC family)

Chain O: 




- Molecule 1: Transcriptional regulator (NtrC family)

Chain P: 




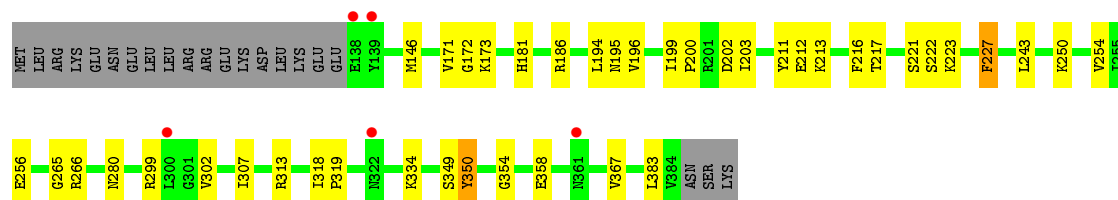
- Molecule 1: Transcriptional regulator (NtrC family)

Chain Q: 




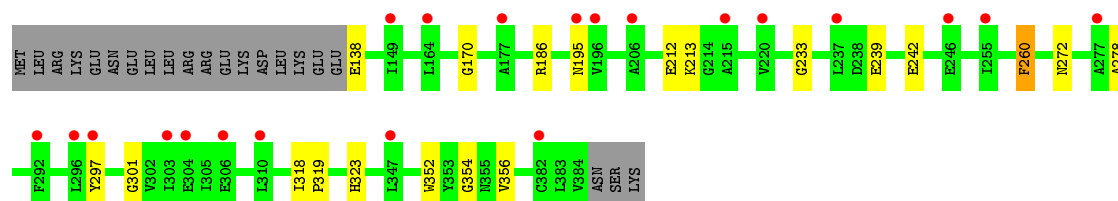
- Molecule 1: Transcriptional regulator (NtrC family)

Chain R: 

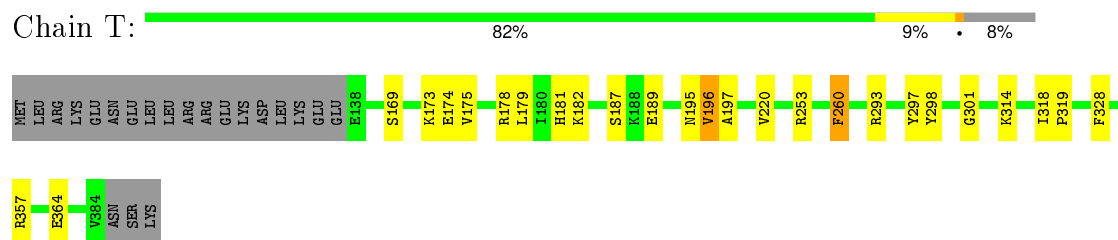


- Molecule 1: Transcriptional regulator (NtrC family)

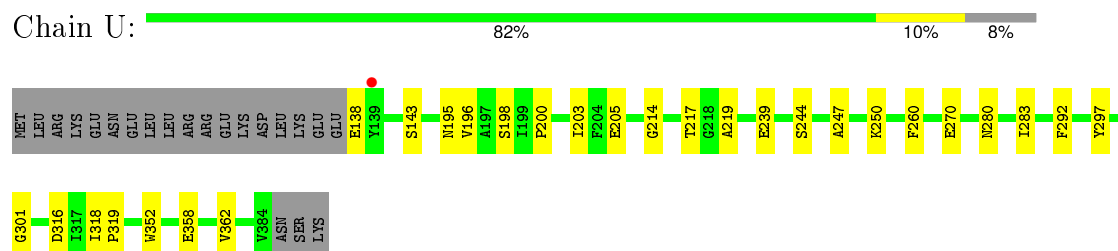
Chain S: 



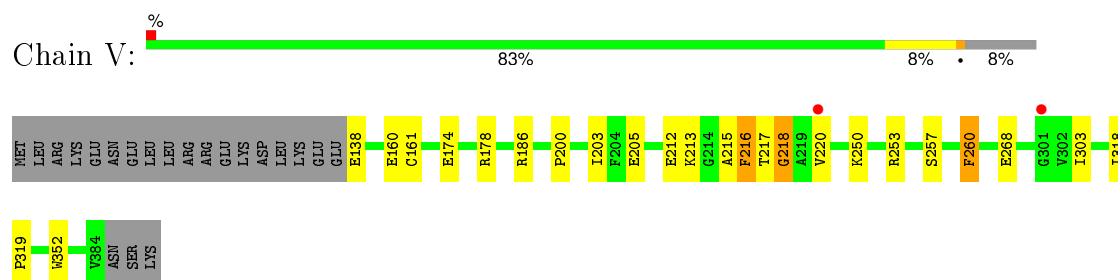
- Molecule 1: Transcriptional regulator (NtrC family)



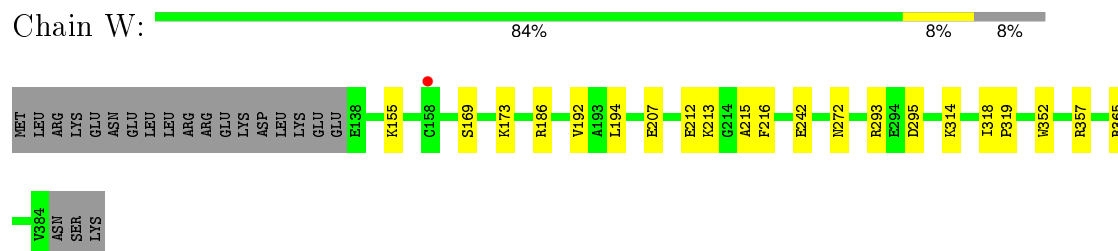
- Molecule 1: Transcriptional regulator (NtrC family)



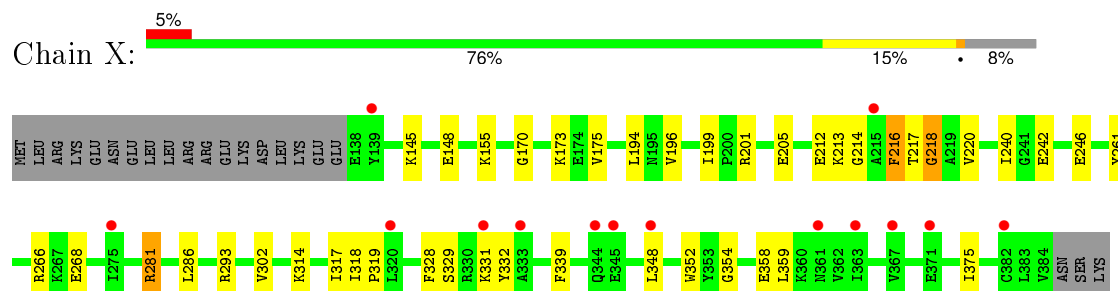
- Molecule 1: Transcriptional regulator (NtrC family)



- 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 3.56Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.258 , 0.308 0.270 , 0.310	Depositor DCC
R_{free} test set	5533 reflections (5.73%)	DCC
Wilson B-factor (Å ²)	86.8	Xtriage
Anisotropy	0.943	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 72.9	EDS
Estimated twinning fraction	0.237 for h,-k,-l 0.319 for -h,k,-l 0.219 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 109790 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	97439	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.24	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.

All (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
1	N	215	ALA	Peptide
1	O	216	PHE	Peptide
1	U	214	GLY	Peptide
1	V	216	PHE	Peptide
1	V	218	GLY	Peptide
1	X	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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.

All (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
1:P:213:LYS:NZ	1:U:270:GLU:O	2.15	0.80
1:I:205:GLU:OE2	1:I:250:LYS:NZ	2.15	0.79
1:O:205:GLU:OE2	1:O:250:LYS:NZ	2.18	0.76
1:V:216:PHE:O	1:V:218:GLY:N	2.18	0.75
1:L:205:GLU:OE2	1:L:250:LYS:NZ	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:205:GLU:OE1	1:P:250:LYS:NZ	2.20	0.74
1:R:334:LYS:NZ	1:R:367:VAL:O	2.20	0.74
1:D:242:GLU:OE1	1:D:281:ARG:NE	2.21	0.74
1:O:280:ASN:ND2	2:O:400:08T:F3	2.12	0.73
1:W:242:GLU:OE2	1:X:293:ARG:NH2	2.21	0.73
1:P:365:ARG:NE	1:Q:302:VAL:O	2.21	0.72
1:F:334:LYS:NZ	1:F:367:VAL:O	2.24	0.71
1:U:205:GLU:OE2	1:U:250:LYS:NZ	2.19	0.71
1:J:205:GLU:OE1	1:J:250:LYS:NZ	2.23	0.69
1:L:357:ARG:NH2	4:L:400:ADP:O1B	2.24	0.69
1:F:168:GLU:O	1:F:173:LYS:NZ	2.24	0.69
1:J:217:THR:O	1:J:219:ALA:N	2.25	0.69
1:T:173:LYS:NZ	2:T:400:08T:O1B	2.17	0.69
1:M:145:LYS:NZ	1:M:312:GLU:O	2.25	0.69
1:E:173:LYS:NZ	2:E:400:08T:O2B	2.23	0.68
1:S:242:GLU:OE2	1:T:293:ARG:NH2	2.27	0.68
1:E:242:GLU:OE1	1:F:293:ARG:NH1	2.27	0.68
1:D:173:LYS:NZ	2:D:400:08T:O2B	2.26	0.67
1:V:215:ALA:HB3	1:V:216:PHE:HB2	1.76	0.67
1:P:242:GLU:OE1	1:P:281:ARG:NE	2.28	0.67
1:N:168:GLU:O	1:N:173:LYS:NZ	2.27	0.67
1:D:205:GLU:OE1	1:D:250:LYS:NZ	2.28	0.66
1:D:365:ARG:NE	1:E:302:VAL:O	2.28	0.66
1:A:138:GLU:N	1:A:138:GLU:OE2	2.28	0.66
1:S:186:ARG:NH1	1:S:233:GLY:O	2.27	0.66
1:I:166:THR:OG1	1:I:306:GLU:OE2	2.13	0.66
1:V:174:GLU:OE2	1:V:178:ARG:NH1	2.28	0.66
1:E:173:LYS:N	2:E:400:08T:O1A	2.29	0.65
1:E:280:ASN:OD1	1:E:281:ARG:NH1	2.29	0.65
1:G:173:LYS:NZ	2:G:400:08T:O2B	2.22	0.65
1:D:215:ALA:O	1:D:217:THR:N	2.29	0.65
1:M:242:GLU:OE2	1:N:293:ARG:NH1	2.28	0.64
1:O:166:THR:OG1	1:O:306:GLU:OE2	2.15	0.64
1:I:169:SER:OG	1:I:357:ARG:NH1	2.30	0.64
1:J:174:GLU:OE2	1:J:178:ARG:NH1	2.29	0.64
1:R:146:MET:SD	1:R:313:ARG:NH2	2.71	0.63
1:H:205:GLU:OE2	1:H:250:LYS:NZ	2.32	0.63
1:P:253:ARG:O	1:P:257:SER:OG	2.15	0.63
1:A:205:GLU:OE1	1:A:250:LYS:NZ	2.32	0.62
1:P:215:ALA:O	1:P:216:PHE:HB2	1.99	0.61
1:J:314:LYS:NZ	1:J:348:LEU:O	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:SER:O	1:B:355:ASN:ND2	2.30	0.61
1:E:239:GLU:OE2	1:E:280:ASN:ND2	2.34	0.60
1:U:195:ASN:ND2	1:U:239:GLU:OE2	2.34	0.60
1:M:297:TYR:O	1:M:301:GLY:N	2.34	0.60
1:W:186:ARG:NH2	1:W:272:ASN:OD1	2.35	0.60
1:M:138:GLU:N	1:M:138:GLU:OE2	2.34	0.60
1:C:138:GLU:OE2	1:C:138:GLU:N	2.35	0.60
1:F:283:ILE:HG23	1:F:284:LYS:H	1.67	0.59
1:F:202:ASP:OD1	1:F:203:ILE:N	2.34	0.59
1:O:138:GLU:N	1:O:138:GLU:OE2	2.36	0.59
1:O:173:LYS:NZ	2:O:400:08T:O1B	2.34	0.59
1:L:354:GLY:HA3	1:L:358:GLU:HB2	1.83	0.59
1:V:160:GLU:OE2	1:V:186:ARG:NH2	2.36	0.58
1:S:138:GLU:N	1:S:138:GLU:OE2	2.37	0.58
1:G:138:GLU:OE2	1:G:138:GLU:N	2.36	0.58
1:C:203:ILE:HG21	1:D:215:ALA:HB1	1.84	0.58
1:A:297:TYR:O	1:A:301:GLY:N	2.36	0.58
1:R:213:LYS:N	1:R:222:SER:OG	2.37	0.58
1:G:357:ARG:NH2	2:G:400:08T:O1B	2.34	0.57
1:V:138:GLU:OE2	1:V:138:GLU:N	2.37	0.57
1:C:202:ASP:OD1	1:C:203:ILE:N	2.37	0.57
1:P:168:GLU:O	1:P:173:LYS:NZ	2.38	0.57
1:D:253:ARG:O	1:D:257:SER:OG	2.21	0.57
1:K:186:ARG:NH2	1:K:272:ASN:OD1	2.37	0.57
1:X:155:LYS:HA	1:X:155:LYS:HE2	1.87	0.57
1:U:138:GLU:N	1:U:138:GLU:OE2	2.38	0.57
1:Q:159:ALA:O	1:Q:274:ARG:NH1	2.37	0.57
1:O:173:LYS:N	2:O:400:08T:O1A	2.38	0.57
1:G:186:ARG:NH1	1:G:233:GLY:O	2.38	0.56
1:N:173:LYS:N	2:N:400:08T:O1A	2.38	0.56
1:M:168:GLU:O	1:M:173:LYS:NZ	2.38	0.56
1:C:173:LYS:NZ	1:C:279:THR:O	2.37	0.56
1:D:138:GLU:OE2	1:D:138:GLU:N	2.38	0.56
1:I:138:GLU:N	1:I:138:GLU:OE2	2.39	0.56
1:J:138:GLU:N	1:J:138:GLU:OE2	2.38	0.56
1:D:202:ASP:OD1	1:D:203:ILE:N	2.39	0.56
1:Q:242:GLU:OE1	1:Q:281:ARG:NH2	2.38	0.56
1:F:216:PHE:HB3	1:F:217:THR:HB	1.89	0.55
1:E:361:ASN:ND2	1:F:298:TYR:O	2.40	0.55
1:I:169:SER:O	1:I:355:ASN:ND2	2.39	0.55
1:P:217:THR:O	1:P:217:THR:OG1	2.24	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:171:VAL:HG12	1:F:355:ASN:CB	2.37	0.54
1:I:242:GLU:OE2	1:I:281:ARG:NH1	2.41	0.54
1:O:216:PHE:HB3	1:P:217:THR:HG22	1.89	0.54
1:M:173:LYS:NZ	2:M:400:08T:O2B	2.26	0.54
1:O:175:VAL:O	1:O:179:LEU:N	2.41	0.54
1:N:172:GLY:HA2	2:N:400:08T:H14	1.90	0.53
1:E:173:LYS:H	2:E:400:08T:H9	1.55	0.53
1:J:253:ARG:O	1:J:257:SER:OG	2.24	0.53
1:A:169:SER:CB	2:A:400:08T:F3	2.31	0.53
1:G:297:TYR:O	1:G:301:GLY:N	2.41	0.53
1:P:365:ARG:NH2	1:Q:301:GLY:O	2.40	0.52
1:F:253:ARG:O	1:F:257:SER:OG	2.26	0.52
1:I:186:ARG:NH1	1:I:272:ASN:OD1	2.42	0.52
1:K:365:ARG:NH2	1:L:302:VAL:O	2.43	0.52
1:J:253:ARG:NH2	1:J:268:GLU:OE2	2.43	0.52
1:K:155:LYS:HE2	1:K:155:LYS:HA	1.92	0.52
1:O:168:GLU:O	1:O:173:LYS:NZ	2.43	0.51
1:D:357:ARG:NH2	2:D:400:08T:O3A	2.43	0.51
1:R:202:ASP:OD1	1:R:203:ILE:N	2.42	0.51
1:O:169:SER:O	1:O:355:ASN:ND2	2.39	0.51
1:Q:155:LYS:HA	1:Q:155:LYS:HE2	1.92	0.51
1:J:284:LYS:NZ	1:J:297:TYR:OH	2.33	0.51
1:B:166:THR:OG1	1:B:306:GLU:OE1	2.22	0.51
1:F:216:PHE:HB3	1:F:217:THR:C	2.31	0.51
1:V:200:PRO:HG2	1:V:203:ILE:HG12	1.93	0.51
1:P:212:GLU:HG3	1:P:213:LYS:H	1.76	0.51
1:I:253:ARG:O	1:I:257:SER:OG	2.25	0.50
1:L:155:LYS:HE2	1:L:155:LYS:HA	1.93	0.50
1:L:216:PHE:HA	1:L:217:THR:HB	1.93	0.50
1:C:358:GLU:O	1:C:362:VAL:N	2.38	0.50
1:X:242:GLU:OE1	1:X:281:ARG:NH2	2.44	0.50
1:T:169:SER:OG	1:T:357:ARG:NH1	2.45	0.50
2:J:400:08T:PA	2:J:400:08T:H4	2.52	0.50
1:B:173:LYS:N	2:B:400:08T:O2A	2.45	0.50
1:L:221:SER:OG	1:L:222:SER:N	2.45	0.49
1:F:242:GLU:OE2	1:F:280:ASN:ND2	2.46	0.49
1:E:155:LYS:HA	1:E:155:LYS:HE2	1.95	0.49
1:L:216:PHE:HA	1:L:217:THR:CB	2.43	0.49
1:H:357:ARG:NH2	2:H:400:08T:O3A	2.45	0.48
1:H:195:ASN:O	1:H:196:VAL:HG12	2.12	0.48
1:B:195:ASN:O	1:B:196:VAL:HG12	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:GLU:O	1:A:173:LYS:NZ	2.46	0.48
1:V:253:ARG:O	1:V:257:SER:OG	2.25	0.48
1:W:155:LYS:HA	1:W:155:LYS:HE2	1.94	0.48
1:Q:332:TYR:OH	1:Q:364:GLU:OE2	2.31	0.48
1:R:171:VAL:O	1:R:173:LYS:N	2.46	0.48
1:T:195:ASN:O	1:T:196:VAL:HG12	2.13	0.48
1:N:195:ASN:O	1:N:196:VAL:HG12	2.14	0.48
1:A:245:LEU:HB2	1:F:200:PRO:HG3	1.96	0.48
1:T:181:HIS:NE2	1:T:189:GLU:O	2.46	0.48
1:E:242:GLU:OE2	1:F:293:ARG:NH2	2.47	0.47
1:M:173:LYS:N	2:M:400:08T:O2A	2.47	0.47
1:G:170:GLY:N	2:G:400:08T:O1B	2.48	0.47
1:W:293:ARG:NE	1:W:295:ASP:OD2	2.42	0.47
1:R:171:VAL:O	1:R:171:VAL:HG23	2.14	0.47
1:D:206:ALA:HB2	1:D:216:PHE:CE2	2.50	0.47
1:P:204:PHE:HE2	1:P:247:ALA:HB1	1.80	0.47
1:X:354:GLY:HA3	1:X:358:GLU:HB2	1.96	0.47
1:C:200:PRO:HG2	1:C:203:ILE:HG12	1.96	0.47
1:G:212:GLU:HG3	1:G:213:LYS:H	1.80	0.47
1:M:212:GLU:HG3	1:M:213:LYS:H	1.79	0.47
1:L:172:GLY:N	4:L:400:ADP:O1A	2.39	0.47
1:J:200:PRO:HG2	1:J:203:ILE:HG12	1.97	0.47
1:S:195:ASN:HB2	1:T:253:ARG:HD2	1.97	0.47
1:X:216:PHE:CB	1:X:218:GLY:N	2.78	0.47
1:K:357:ARG:NH2	2:K:400:08T:O3A	2.47	0.47
1:T:182:LYS:O	1:T:187:SER:OG	2.24	0.47
1:I:159:ALA:O	1:I:274:ARG:NH1	2.48	0.46
1:N:318:ILE:N	1:N:319:PRO:CD	2.78	0.46
1:D:174:GLU:OE2	1:D:178:ARG:NH1	2.48	0.46
1:R:200:PRO:HD2	1:R:203:ILE:HD11	1.97	0.46
1:W:318:ILE:N	1:W:319:PRO:CD	2.79	0.46
1:F:171:VAL:HG12	1:F:355:ASN:HB2	1.97	0.46
1:R:318:ILE:HB	1:R:319:PRO:HD3	1.97	0.46
1:V:212:GLU:HG3	1:V:213:LYS:H	1.80	0.46
1:W:212:GLU:HG3	1:W:213:LYS:N	2.31	0.46
1:X:212:GLU:O	1:X:214:GLY:N	2.49	0.46
1:D:204:PHE:HE2	1:D:247:ALA:HB1	1.81	0.46
1:Q:216:PHE:HB3	1:Q:218:GLY:H	1.81	0.46
1:K:216:PHE:C	1:K:218:GLY:H	2.18	0.46
1:S:170:GLY:N	2:S:400:08T:O2B	2.43	0.46
1:H:205:GLU:N	1:H:205:GLU:OE1	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:176:VAL:HG21	1:J:307:ILE:HD11	1.98	0.46
1:A:250:LYS:O	1:A:251:LEU:HB3	2.16	0.45
1:L:340:THR:HG22	1:L:374:PHE:HB3	1.98	0.45
1:B:212:GLU:HG3	1:B:213:LYS:H	1.81	0.45
1:V:215:ALA:HB3	1:V:216:PHE:CB	2.45	0.45
1:D:200:PRO:HG2	1:D:203:ILE:HG12	1.97	0.45
1:G:184:SER:O	1:G:187:SER:OG	2.33	0.45
1:K:212:GLU:HG3	1:K:213:LYS:H	1.81	0.45
1:J:173:LYS:NZ	2:J:400:08T:O1B	2.40	0.45
1:J:200:PRO:HG2	1:J:203:ILE:CG1	2.47	0.45
1:X:201:ARG:NH1	1:X:246:GLU:OE1	2.48	0.45
1:Q:318:ILE:N	1:Q:319:PRO:CD	2.79	0.45
1:W:192:VAL:HG12	1:W:194:LEU:CD1	2.46	0.45
1:T:328:PHE:CE2	1:T:364:GLU:HB2	2.51	0.45
1:C:166:THR:OG1	1:C:306:GLU:OE2	2.33	0.45
1:E:194:LEU:HD21	1:E:226:PHE:CD2	2.52	0.45
1:Q:198:SER:HA	1:R:250:LYS:HD3	1.98	0.45
1:R:349:SER:O	1:R:350:TYR:HB2	2.17	0.45
1:X:281:ARG:HG2	1:X:286:LEU:HD11	1.98	0.45
1:E:318:ILE:N	1:E:319:PRO:CD	2.80	0.45
1:X:216:PHE:HB3	1:X:217:THR:HB	1.97	0.45
1:F:171:VAL:O	1:F:171:VAL:HG23	2.17	0.45
1:S:318:ILE:N	1:S:319:PRO:CD	2.80	0.45
1:X:328:PHE:O	1:X:331:LYS:N	2.50	0.45
1:C:283:ILE:HD11	1:C:292:PHE:CE2	2.52	0.45
1:N:212:GLU:HG3	1:N:213:LYS:H	1.82	0.45
1:V:253:ARG:NH2	1:V:268:GLU:OE2	2.50	0.45
1:X:314:LYS:HB3	1:X:348:LEU:HD22	1.98	0.45
1:P:324:PHE:CD2	1:P:360:LYS:HA	2.52	0.45
1:V:200:PRO:HG2	1:V:203:ILE:CG1	2.47	0.44
1:E:192:VAL:HG12	1:E:194:LEU:CD1	2.47	0.44
1:P:223:LYS:HD3	1:Q:264:GLY:O	2.17	0.44
1:B:195:ASN:C	1:B:197:ALA:H	2.20	0.44
1:J:169:SER:O	1:J:355:ASN:ND2	2.49	0.44
1:E:365:ARG:NH1	1:E:383:LEU:HG	2.32	0.44
1:U:244:SER:O	1:U:247:ALA:N	2.50	0.44
1:P:232:GLY:HA3	1:T:220:VAL:HG21	1.99	0.44
1:O:174:GLU:N	2:O:400:08T:O1A	2.37	0.44
1:U:200:PRO:HG2	1:U:203:ILE:CG1	2.47	0.44
1:C:318:ILE:N	1:C:319:PRO:CD	2.80	0.44
1:P:283:ILE:HD11	1:P:292:PHE:CE2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:317:ILE:HD12	1:X:348:LEU:HD23	2.00	0.44
1:X:196:VAL:HG11	1:X:240:ILE:HD13	1.98	0.44
1:D:260:PHE:CD1	1:D:260:PHE:C	2.91	0.44
1:X:205:GLU:OE1	1:X:205:GLU:N	2.50	0.44
1:K:194:LEU:HD21	1:K:226:PHE:CD2	2.53	0.44
1:O:216:PHE:CG	1:P:217:THR:HG22	2.53	0.44
1:P:285:GLU:HA	1:P:288:LYS:HE3	2.00	0.44
1:X:261:TYR:CZ	1:X:268:GLU:HG3	2.53	0.44
1:H:318:ILE:N	1:H:319:PRO:CD	2.80	0.44
1:F:159:ALA:O	1:F:274:ARG:NH1	2.50	0.44
1:T:174:GLU:OE1	1:T:178:ARG:NH1	2.51	0.44
1:W:357:ARG:NH2	2:W:400:08T:O3A	2.51	0.44
1:B:186:ARG:NH2	1:B:272:ASN:OD1	2.43	0.44
1:X:175:VAL:HG21	4:X:400:ADP:C5	2.53	0.44
1:X:173:LYS:NZ	4:X:400:ADP:O1B	2.48	0.44
1:A:354:GLY:HA2	1:B:298:TYR:CE2	2.53	0.44
1:O:283:ILE:HD11	1:O:292:PHE:CD2	2.53	0.44
1:J:217:THR:C	1:J:219:ALA:H	2.20	0.43
1:G:238:ASP:OD2	2:G:400:08T:F2	2.26	0.43
1:D:318:ILE:N	1:D:319:PRO:CD	2.81	0.43
1:G:207:GLU:OE1	1:H:264:GLY:N	2.50	0.43
1:T:195:ASN:C	1:T:197:ALA:H	2.21	0.43
1:V:260:PHE:CD1	1:V:260:PHE:C	2.91	0.43
1:S:138:GLU:O	1:S:323:HIS:NE2	2.51	0.43
1:R:212:GLU:HG3	1:R:213:LYS:H	1.83	0.43
1:R:199:ILE:HA	1:R:200:PRO:HD3	1.91	0.43
1:P:318:ILE:N	1:P:319:PRO:CD	2.81	0.43
1:X:216:PHE:HB3	1:X:218:GLY:N	2.33	0.43
1:R:196:VAL:HG21	1:R:243:LEU:HD22	2.00	0.43
1:O:200:PRO:HG2	1:O:203:ILE:HG12	1.99	0.43
1:T:318:ILE:N	1:T:319:PRO:CD	2.82	0.43
1:F:216:PHE:HB3	1:F:218:GLY:N	2.34	0.43
1:X:145:LYS:O	1:X:148:GLU:HG2	2.19	0.43
1:G:318:ILE:N	1:G:319:PRO:CD	2.80	0.43
1:R:265:GLY:O	1:R:266:ARG:HD3	2.19	0.43
1:D:365:ARG:NH2	1:E:301:GLY:O	2.50	0.43
1:W:207:GLU:HA	1:X:266:ARG:HH22	1.83	0.43
1:N:169:SER:O	1:N:355:ASN:ND2	2.46	0.43
1:M:184:SER:O	1:M:187:SER:OG	2.37	0.43
1:U:297:TYR:O	1:U:301:GLY:N	2.52	0.43
1:M:318:ILE:N	1:M:319:PRO:CD	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:215:ALA:O	1:K:216:PHE:HB2	2.19	0.43
1:X:317:ILE:HG23	1:X:359:LEU:HD11	2.00	0.43
1:J:361:ASN:ND2	1:K:298:TYR:O	2.51	0.43
1:H:207:GLU:OE1	1:I:264:GLY:N	2.50	0.43
1:P:198:SER:HA	1:Q:250:LYS:HD3	2.00	0.43
1:B:318:ILE:N	1:B:319:PRO:CD	2.82	0.43
1:O:212:GLU:HG3	1:O:213:LYS:H	1.83	0.43
1:O:174:GLU:HB3	2:O:400:08T:O2A	2.19	0.43
1:N:186:ARG:NH2	1:N:272:ASN:OD1	2.50	0.43
1:J:168:GLU:HB2	1:J:355:ASN:HD21	1.84	0.42
1:J:318:ILE:N	1:J:319:PRO:CD	2.82	0.42
1:M:292:PHE:CE1	1:M:296:LEU:HD23	2.54	0.42
1:K:318:ILE:N	1:K:319:PRO:CD	2.82	0.42
1:E:328:PHE:CE2	1:E:364:GLU:HB2	2.54	0.42
1:M:200:PRO:HD2	1:M:203:ILE:HD11	2.01	0.42
1:L:318:ILE:N	1:L:319:PRO:CD	2.82	0.42
1:F:283:ILE:HG13	1:F:284:LYS:N	2.33	0.42
1:O:318:ILE:N	1:O:319:PRO:CD	2.82	0.42
1:G:215:ALA:CB	1:G:264:GLY:HA3	2.49	0.42
1:G:366:ALA:O	1:G:370:SER:N	2.52	0.42
1:I:354:GLY:HA3	1:I:358:GLU:HB2	2.00	0.42
1:I:297:TYR:O	1:I:301:GLY:N	2.52	0.42
1:U:196:VAL:HG13	1:U:196:VAL:O	2.20	0.42
1:S:239:GLU:N	1:S:278:ALA:O	2.52	0.42
1:H:195:ASN:ND2	1:I:249:ALA:O	2.49	0.42
1:X:314:LYS:HD3	1:X:348:LEU:HB3	2.01	0.42
1:O:283:ILE:HD11	1:O:292:PHE:CE2	2.54	0.42
1:I:318:ILE:N	1:I:319:PRO:CD	2.82	0.42
1:O:217:THR:C	1:O:219:ALA:H	2.22	0.42
1:F:194:LEU:HD22	1:F:226:PHE:CD2	2.54	0.42
1:L:283:ILE:HD11	1:L:292:PHE:CE2	2.55	0.42
1:O:174:GLU:H	2:O:400:08T:H9	1.59	0.42
1:X:339:PHE:HA	1:X:375:ILE:H	1.84	0.42
1:H:253:ARG:HB2	1:H:253:ARG:NH1	2.34	0.42
1:Q:192:VAL:HG12	1:Q:194:LEU:CD1	2.50	0.42
1:S:356:VAL:CG1	2:S:400:08T:H8	2.50	0.42
1:O:354:GLY:HA3	1:O:358:GLU:HB2	2.02	0.42
1:L:317:ILE:HD12	1:L:348:LEU:HD23	2.01	0.42
1:P:174:GLU:HB3	2:P:400:08T:O2A	2.19	0.42
1:H:176:VAL:HG21	1:H:307:ILE:HD11	2.02	0.42
1:V:161:CYS:SG	1:V:303:ILE:HD11	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:ILE:N	1:A:319:PRO:CD	2.83	0.42
1:O:172:GLY:HA3	2:O:400:08T:H10	2.01	0.42
1:V:318:ILE:N	1:V:319:PRO:CD	2.82	0.42
1:H:328:PHE:CE2	1:H:364:GLU:HB2	2.55	0.42
1:L:305:ILE:HG22	1:L:307:ILE:HG12	2.02	0.42
1:A:143:SER:N	1:A:316:ASP:OD1	2.47	0.42
1:Q:328:PHE:CE2	1:Q:364:GLU:HB2	2.55	0.41
1:F:184:SER:OG	1:F:185:ASP:N	2.53	0.41
1:S:260:PHE:CD1	1:S:260:PHE:C	2.93	0.41
1:O:245:LEU:HD12	1:O:245:LEU:H	1.84	0.41
1:R:181:HIS:NE2	1:R:186:ARG:O	2.53	0.41
1:X:216:PHE:HB2	1:X:218:GLY:N	2.35	0.41
1:R:194:LEU:HD23	1:R:195:ASN:N	2.35	0.41
1:S:297:TYR:O	1:S:301:GLY:N	2.51	0.41
1:D:195:ASN:ND2	1:D:198:SER:OG	2.47	0.41
1:A:234:THR:HG23	1:A:276:LEU:HD13	2.02	0.41
1:D:280:ASN:ND2	2:D:400:08T:F3	2.40	0.41
1:X:170:GLY:N	4:X:400:ADP:O3B	2.53	0.41
1:R:227:PHE:CE2	1:R:254:VAL:HG11	2.55	0.41
1:X:352:TRP:CZ3	1:X:359:LEU:HA	2.56	0.41
1:X:194:LEU:HD21	1:X:199:ILE:HD11	2.02	0.41
1:U:217:THR:C	1:U:219:ALA:H	2.24	0.41
1:C:217:THR:C	1:C:219:ALA:H	2.24	0.41
1:F:171:VAL:O	1:F:173:LYS:N	2.53	0.41
1:Q:216:PHE:O	1:Q:217:THR:CB	2.68	0.41
1:M:196:VAL:O	1:M:196:VAL:HG13	2.20	0.41
1:D:283:ILE:HD11	1:D:292:PHE:CE2	2.56	0.41
1:L:139:TYR:CE1	1:L:175:VAL:HG13	2.55	0.41
1:I:212:GLU:HG3	1:I:213:LYS:H	1.85	0.41
1:S:186:ARG:NH2	1:S:272:ASN:OD1	2.47	0.41
1:A:170:GLY:H	2:A:400:08T:PB	2.44	0.41
1:K:215:ALA:O	1:K:216:PHE:CB	2.68	0.41
1:W:169:SER:HA	1:W:173:LYS:HZ1	1.85	0.41
1:R:354:GLY:HA3	1:R:358:GLU:HB2	2.03	0.41
1:P:232:GLY:HA3	1:T:220:VAL:CB	2.50	0.41
1:O:200:PRO:HG2	1:O:203:ILE:CG1	2.50	0.41
1:T:260:PHE:C	1:T:260:PHE:CD1	2.94	0.41
1:C:212:GLU:HG3	1:C:213:LYS:H	1.85	0.41
1:U:318:ILE:N	1:U:319:PRO:CD	2.83	0.41
1:E:207:GLU:OE1	1:F:264:GLY:N	2.48	0.41
1:L:356:VAL:O	1:L:356:VAL:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:198:SER:HA	1:V:250:LYS:HD3	2.03	0.41
1:K:313:ARG:O	1:K:315:GLU:N	2.54	0.41
1:O:297:TYR:O	1:O:301:GLY:N	2.54	0.41
1:M:186:ARG:NH1	1:M:233:GLY:O	2.53	0.41
1:J:198:SER:HA	1:K:250:LYS:HD3	2.02	0.41
1:P:216:PHE:C	1:P:217:THR:HG23	2.42	0.40
1:F:216:PHE:CB	1:F:218:GLY:N	2.84	0.40
1:X:216:PHE:HB3	1:X:217:THR:C	2.42	0.40
1:K:192:VAL:HG12	1:K:194:LEU:CD1	2.50	0.40
1:U:358:GLU:O	1:U:362:VAL:N	2.46	0.40
1:A:283:ILE:HD11	1:A:292:PHE:CD2	2.55	0.40
1:M:216:PHE:CZ	1:R:221:SER:HB3	2.55	0.40
1:I:196:VAL:O	1:I:196:VAL:HG13	2.22	0.40
1:Q:365:ARG:NE	1:R:302:VAL:O	2.54	0.40
1:Q:166:THR:HG22	1:Q:167:GLY:N	2.36	0.40
1:U:143:SER:N	1:U:316:ASP:OD1	2.41	0.40
1:R:256:GLU:HB2	1:R:299:ARG:HE	1.85	0.40
1:T:175:VAL:O	1:T:179:LEU:N	2.53	0.40
1:W:365:ARG:NE	1:X:302:VAL:O	2.55	0.40
1:R:211:TYR:CZ	1:R:223:LYS:HB2	2.57	0.40
1:S:212:GLU:HG3	1:S:213:LYS:H	1.86	0.40
1:C:196:VAL:O	1:C:196:VAL:HG13	2.21	0.40
1:K:260:PHE:CD1	1:K:260:PHE:C	2.95	0.40
1:I:245:LEU:HD12	1:I:245:LEU:H	1.86	0.40
1:M:243:LEU:HD23	1:M:248:GLN:HG2	2.04	0.40
1:G:168:GLU:O	1:G:173:LYS:NZ	2.54	0.40
1:H:195:ASN:C	1:H:197:ALA:H	2.24	0.40
1:J:204:PHE:HE2	1:J:247:ALA:HB1	1.86	0.40
1:P:328:PHE:CE2	1:P:364:GLU:HB2	2.57	0.40
1:A:354:GLY:HA3	1:A:358:GLU:HB2	2.03	0.40
1:D:283:ILE:HD11	1:D:292:PHE:CD2	2.57	0.40
1:U:283:ILE:HD11	1:U:292:PHE:CE2	2.57	0.40
1:P:297:TYR:O	1:P:301:GLY:N	2.54	0.40
1:D:161:CYS:SG	1:D:303:ILE:HD11	2.61	0.40
1:O:244:SER:O	1:O:247:ALA:N	2.53	0.40
1:X:318:ILE:HB	1:X:319:PRO:HD3	2.02	0.40
1:T:297:TYR:O	1:T:301:GLY:N	2.53	0.40
1:S:354:GLY:HA2	1:T:298:TYR:CE2	2.57	0.40
1:O:196:VAL:HG13	1:O:196:VAL:O	2.22	0.40
1:J:366:ALA:O	1:J:370:SER:N	2.55	0.40
1:E:260:PHE:CE1	1:E:269:ILE:HB	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:297:TYR:O	1:H:301:GLY:N	2.54	0.40
1:L:173:LYS:N	4:L:400:ADP:O2A	2.54	0.40
1:P:206:ALA:HB2	1:P:216:PHE:HE2	1.86	0.40
1:J:365:ARG:NE	1:K:302:VAL:O	2.37	0.40

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	245/268 (91%)	232 (95%)	12 (5%)	1 (0%)	39	80
1	B	245/268 (91%)	231 (94%)	13 (5%)	1 (0%)	39	80
1	C	245/268 (91%)	230 (94%)	14 (6%)	1 (0%)	39	80
1	D	245/268 (91%)	228 (93%)	14 (6%)	3 (1%)	16	62
1	E	245/268 (91%)	230 (94%)	13 (5%)	2 (1%)	24	69
1	F	245/268 (91%)	221 (90%)	20 (8%)	4 (2%)	12	56
1	G	245/268 (91%)	230 (94%)	14 (6%)	1 (0%)	39	80
1	H	245/268 (91%)	230 (94%)	13 (5%)	2 (1%)	24	69
1	I	245/268 (91%)	233 (95%)	11 (4%)	1 (0%)	39	80
1	J	245/268 (91%)	230 (94%)	12 (5%)	3 (1%)	16	62
1	K	245/268 (91%)	227 (93%)	15 (6%)	3 (1%)	16	62
1	L	245/268 (91%)	226 (92%)	17 (7%)	2 (1%)	24	69
1	M	245/268 (91%)	229 (94%)	15 (6%)	1 (0%)	39	80
1	N	245/268 (91%)	231 (94%)	12 (5%)	2 (1%)	24	69
1	O	245/268 (91%)	230 (94%)	14 (6%)	1 (0%)	39	80
1	P	245/268 (91%)	230 (94%)	13 (5%)	2 (1%)	24	69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	245/268 (91%)	228 (93%)	14 (6%)	3 (1%)	16	62
1	R	245/268 (91%)	235 (96%)	6 (2%)	4 (2%)	12	56
1	S	245/268 (91%)	232 (95%)	12 (5%)	1 (0%)	39	80
1	T	245/268 (91%)	229 (94%)	14 (6%)	2 (1%)	24	69
1	U	245/268 (91%)	230 (94%)	14 (6%)	1 (0%)	39	80
1	V	245/268 (91%)	228 (93%)	14 (6%)	3 (1%)	16	62
1	W	245/268 (91%)	229 (94%)	13 (5%)	3 (1%)	16	62
1	X	245/268 (91%)	234 (96%)	8 (3%)	3 (1%)	16	62
All	All	5880/6432 (91%)	5513 (94%)	317 (5%)	50 (1%)	21	67

All (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
1	R	217	THR
1	R	307	ILE
1	T	196	VAL
1	V	217	THR
1	X	213	LYS
1	D	216	PHE
1	J	218	GLY
1	K	216	PHE
1	R	172	GLY
1	W	215	ALA
1	X	329	SER
1	F	215	ALA
1	F	283	ILE
1	K	314	LYS
1	E	352	TRP
1	G	352	TRP
1	I	352	TRP
1	J	352	TRP
1	L	352	TRP
1	M	352	TRP
1	N	314	LYS

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Mol	Chain	Res	Type
1	Q	314	LYS
1	Q	352	TRP
1	S	352	TRP
1	V	352	TRP
1	W	314	LYS
1	W	352	TRP
1	A	352	TRP
1	C	352	TRP
1	D	352	TRP
1	E	314	LYS
1	H	352	TRP
1	K	352	TRP
1	O	352	TRP
1	P	352	TRP
1	Q	219	ALA
1	T	314	LYS
1	U	352	TRP
1	D	215	ALA
1	F	307	ILE
1	R	350	TYR
1	F	172	GLY
1	L	317	ILE
1	X	220	VAL
1	V	220	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	212/233 (91%)	212 (100%)	0	100	100
1	B	212/233 (91%)	211 (100%)	1 (0%)	92	97
1	C	212/233 (91%)	211 (100%)	1 (0%)	92	97
1	D	212/233 (91%)	209 (99%)	3 (1%)	74	91
1	E	212/233 (91%)	209 (99%)	3 (1%)	74	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	212/233 (91%)	210 (99%)	2 (1%)	84	94
1	G	212/233 (91%)	212 (100%)	0	100	100
1	H	212/233 (91%)	211 (100%)	1 (0%)	92	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%)	92	97
1	L	212/233 (91%)	211 (100%)	1 (0%)	92	97
1	M	212/233 (91%)	211 (100%)	1 (0%)	92	97
1	N	212/233 (91%)	211 (100%)	1 (0%)	92	97
1	O	212/233 (91%)	211 (100%)	1 (0%)	92	97
1	P	212/233 (91%)	209 (99%)	3 (1%)	74	91
1	Q	212/233 (91%)	211 (100%)	1 (0%)	92	97
1	R	212/233 (91%)	208 (98%)	4 (2%)	65	88
1	S	212/233 (91%)	211 (100%)	1 (0%)	92	97
1	T	212/233 (91%)	211 (100%)	1 (0%)	92	97
1	U	212/233 (91%)	210 (99%)	2 (1%)	84	94
1	V	212/233 (91%)	211 (100%)	1 (0%)	92	97
1	W	212/233 (91%)	211 (100%)	1 (0%)	92	97
1	X	212/233 (91%)	210 (99%)	2 (1%)	84	94
All	All	5088/5592 (91%)	5056 (99%)	32 (1%)	90	97

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	260	PHE
1	C	260	PHE
1	D	213	LYS
1	D	216	PHE
1	D	260	PHE
1	E	145	LYS
1	E	216	PHE
1	E	260	PHE
1	F	260	PHE
1	F	280	ASN
1	H	260	PHE

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Mol	Chain	Res	Type
1	K	260	PHE
1	L	260	PHE
1	M	260	PHE
1	N	260	PHE
1	O	280	ASN
1	P	216	PHE
1	P	217	THR
1	P	281	ARG
1	Q	260	PHE
1	R	216	PHE
1	R	227	PHE
1	R	280	ASN
1	R	383	LEU
1	S	260	PHE
1	T	260	PHE
1	U	260	PHE
1	U	280	ASN
1	V	260	PHE
1	W	216	PHE
1	X	281	ARG
1	X	332	TYR

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 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	3.20	9 (34%)	28,52,52	3.12	9 (32%)
2	08T	B	400	3	26,33,33	3.21	9 (34%)	28,52,52	3.02	8 (28%)
2	08T	C	400	3	26,33,33	3.17	9 (34%)	28,52,52	3.04	8 (28%)
2	08T	D	400	3	26,33,33	3.20	9 (34%)	28,52,52	3.08	8 (28%)
2	08T	E	400	3	26,33,33	3.20	9 (34%)	28,52,52	3.13	9 (32%)
2	08T	G	400	3	26,33,33	3.22	9 (34%)	28,52,52	3.12	9 (32%)
2	08T	H	400	1,3	26,33,33	3.23	9 (34%)	28,52,52	3.07	10 (35%)
2	08T	I	400	1,3	26,33,33	3.16	9 (34%)	28,52,52	3.01	8 (28%)
2	08T	J	400	3	26,33,33	3.15	9 (34%)	28,52,52	3.10	10 (35%)
2	08T	K	400	-	26,33,33	3.17	9 (34%)	28,52,52	3.03	9 (32%)
4	ADP	L	400	-	22,29,29	1.00	1 (4%)	27,45,45	1.95	4 (14%)
2	08T	M	400	3	26,33,33	3.17	9 (34%)	28,52,52	3.04	9 (32%)
2	08T	N	400	1,3	26,33,33	3.21	9 (34%)	28,52,52	3.19	10 (35%)
2	08T	O	400	3	26,33,33	3.20	9 (34%)	28,52,52	3.02	10 (35%)
2	08T	P	400	3	26,33,33	3.21	9 (34%)	28,52,52	3.02	8 (28%)
2	08T	Q	400	-	26,33,33	3.18	9 (34%)	28,52,52	3.07	11 (39%)
2	08T	S	400	3	26,33,33	3.20	9 (34%)	28,52,52	3.08	9 (32%)
2	08T	T	400	1,3	26,33,33	3.19	9 (34%)	28,52,52	2.96	10 (35%)
2	08T	U	400	1,3	26,33,33	3.19	9 (34%)	28,52,52	3.02	8 (28%)
2	08T	V	400	3	26,33,33	3.18	9 (34%)	28,52,52	2.96	7 (25%)
2	08T	W	400	3	26,33,33	3.17	9 (34%)	28,52,52	3.03	9 (32%)
4	ADP	X	400	-	22,29,29	0.99	1 (4%)	27,45,45	1.95	4 (14%)

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	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
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

All (182) 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
2	I	400	08T	F2-BE	-7.28	1.35	1.54
2	B	400	08T	F2-BE	-7.28	1.35	1.54
2	V	400	08T	F2-BE	-7.28	1.35	1.54
2	P	400	08T	F2-BE	-7.27	1.35	1.54
2	S	400	08T	F2-BE	-7.25	1.35	1.54
2	A	400	08T	F2-BE	-7.25	1.35	1.54
2	J	400	08T	F2-BE	-7.23	1.35	1.54
2	M	400	08T	F2-BE	-7.23	1.35	1.54
2	C	400	08T	F2-BE	-7.23	1.35	1.54
2	T	400	08T	F2-BE	-7.23	1.35	1.54
2	U	400	08T	F2-BE	-7.23	1.35	1.54
2	E	400	08T	F2-BE	-7.20	1.35	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	400	08T	F2-BE	-7.09	1.36	1.54
2	G	400	08T	F1-BE	-7.04	1.36	1.54
2	K	400	08T	F2-BE	-7.02	1.36	1.54
2	W	400	08T	F2-BE	-6.99	1.36	1.54
2	B	400	08T	F1-BE	-6.85	1.36	1.54
2	A	400	08T	F3-BE	-6.83	1.36	1.54
2	T	400	08T	F1-BE	-6.81	1.36	1.54
2	K	400	08T	F1-BE	-6.77	1.36	1.54
2	O	400	08T	F1-BE	-6.77	1.36	1.54
2	V	400	08T	F1-BE	-6.71	1.36	1.54
2	W	400	08T	F1-BE	-6.71	1.36	1.54
2	D	400	08T	F1-BE	-6.69	1.37	1.54
2	M	400	08T	F1-BE	-6.69	1.37	1.54
2	C	400	08T	F1-BE	-6.69	1.37	1.54
2	Q	400	08T	F1-BE	-6.69	1.37	1.54
2	E	400	08T	F1-BE	-6.69	1.37	1.54
2	P	400	08T	F1-BE	-6.69	1.37	1.54
2	E	400	08T	F3-BE	-6.68	1.37	1.54
2	J	400	08T	F1-BE	-6.68	1.37	1.54
2	U	400	08T	F1-BE	-6.67	1.37	1.54
2	W	400	08T	F3-BE	-6.67	1.37	1.54
2	P	400	08T	F3-BE	-6.65	1.37	1.54
2	H	400	08T	F1-BE	-6.64	1.37	1.54
2	O	400	08T	F3-BE	-6.63	1.37	1.54
2	N	400	08T	F1-BE	-6.63	1.37	1.54
2	A	400	08T	F1-BE	-6.62	1.37	1.54
2	J	400	08T	F3-BE	-6.62	1.37	1.54
2	S	400	08T	F1-BE	-6.62	1.37	1.54
2	K	400	08T	F3-BE	-6.61	1.37	1.54
2	I	400	08T	F1-BE	-6.61	1.37	1.54
2	B	400	08T	F3-BE	-6.60	1.37	1.54
2	D	400	08T	F3-BE	-6.59	1.37	1.54
2	S	400	08T	F3-BE	-6.59	1.37	1.54
2	Q	400	08T	F3-BE	-6.58	1.37	1.54
2	M	400	08T	F3-BE	-6.57	1.37	1.54
2	V	400	08T	F3-BE	-6.57	1.37	1.54
2	H	400	08T	F3-BE	-6.57	1.37	1.54
2	C	400	08T	F3-BE	-6.56	1.37	1.54
2	U	400	08T	F3-BE	-6.56	1.37	1.54
2	G	400	08T	F3-BE	-6.55	1.37	1.54
2	N	400	08T	F3-BE	-6.55	1.37	1.54
2	T	400	08T	F3-BE	-6.47	1.37	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	400	08T	F3-BE	-6.19	1.38	1.54
2	O	400	08T	C5-C4	-4.57	1.30	1.40
2	D	400	08T	C5-C4	-4.53	1.30	1.40
2	S	400	08T	C5-C4	-4.53	1.30	1.40
2	P	400	08T	C5-C4	-4.53	1.30	1.40
2	J	400	08T	C5-C4	-4.51	1.30	1.40
2	A	400	08T	C5-C4	-4.50	1.30	1.40
2	M	400	08T	C5-C4	-4.50	1.30	1.40
2	E	400	08T	C5-C4	-4.50	1.30	1.40
2	G	400	08T	C5-C4	-4.50	1.30	1.40
2	B	400	08T	C5-C4	-4.50	1.30	1.40
2	K	400	08T	C5-C4	-4.49	1.30	1.40
2	Q	400	08T	C5-C4	-4.49	1.30	1.40
2	C	400	08T	C5-C4	-4.48	1.30	1.40
2	U	400	08T	C5-C4	-4.48	1.30	1.40
2	T	400	08T	C5-C4	-4.46	1.30	1.40
2	W	400	08T	C5-C4	-4.46	1.30	1.40
2	V	400	08T	C5-C4	-4.45	1.30	1.40
2	H	400	08T	C5-C4	-4.45	1.30	1.40
2	N	400	08T	C5-C4	-4.40	1.30	1.40
2	I	400	08T	C5-C4	-4.40	1.30	1.40
2	N	400	08T	C5-N7	-3.44	1.27	1.39
2	O	400	08T	C5-N7	-3.44	1.27	1.39
2	B	400	08T	C5-N7	-3.44	1.27	1.39
2	W	400	08T	C5-N7	-3.44	1.27	1.39
2	T	400	08T	C5-N7	-3.43	1.27	1.39
2	I	400	08T	C5-N7	-3.42	1.27	1.39
2	C	400	08T	C5-N7	-3.42	1.27	1.39
2	H	400	08T	C5-N7	-3.42	1.27	1.39
2	V	400	08T	C5-N7	-3.40	1.27	1.39
2	K	400	08T	C5-N7	-3.39	1.27	1.39
2	M	400	08T	C5-N7	-3.39	1.27	1.39
2	U	400	08T	C5-N7	-3.39	1.27	1.39
2	P	400	08T	C5-N7	-3.38	1.27	1.39
2	Q	400	08T	C5-N7	-3.38	1.27	1.39
2	A	400	08T	C5-N7	-3.38	1.27	1.39
2	S	400	08T	C5-N7	-3.38	1.27	1.39
2	G	400	08T	C5-N7	-3.36	1.28	1.39
2	E	400	08T	C5-N7	-3.35	1.28	1.39
2	J	400	08T	C5-N7	-3.35	1.28	1.39
2	D	400	08T	C5-N7	-3.34	1.28	1.39
2	I	400	08T	C2'-C3'	-3.31	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	V	400	08T	C2'-C3'	-3.26	1.44	1.53
2	U	400	08T	C2'-C3'	-3.18	1.44	1.53
2	S	400	08T	C2'-C3'	-3.15	1.44	1.53
2	P	400	08T	C2'-C3'	-3.14	1.44	1.53
2	M	400	08T	C2'-C3'	-3.14	1.44	1.53
2	A	400	08T	C2'-C3'	-3.13	1.44	1.53
2	C	400	08T	C2'-C3'	-3.12	1.44	1.53
2	W	400	08T	C2'-C3'	-3.12	1.44	1.53
2	D	400	08T	C2'-C3'	-3.11	1.44	1.53
2	O	400	08T	C2'-C3'	-3.07	1.45	1.53
2	J	400	08T	C2'-C3'	-3.04	1.45	1.53
2	K	400	08T	C2'-C3'	-3.01	1.45	1.53
2	T	400	08T	C2'-C3'	-3.00	1.45	1.53
2	B	400	08T	C2'-C3'	-2.96	1.45	1.53
2	H	400	08T	C2'-C3'	-2.96	1.45	1.53
2	E	400	08T	C2'-C3'	-2.94	1.45	1.53
2	N	400	08T	C2'-C3'	-2.93	1.45	1.53
2	Q	400	08T	C2'-C3'	-2.93	1.45	1.53
2	G	400	08T	C2'-C3'	-2.90	1.45	1.53
2	O	400	08T	C6-N6	2.37	1.42	1.34
2	J	400	08T	C6-N6	2.52	1.42	1.34
2	A	400	08T	C6-N6	2.55	1.42	1.34
2	M	400	08T	C6-N6	2.56	1.42	1.34
2	S	400	08T	C6-N6	2.56	1.42	1.34
2	G	400	08T	C6-N6	2.56	1.42	1.34
2	K	400	08T	C6-N6	2.57	1.42	1.34
2	C	400	08T	C6-N6	2.57	1.42	1.34
2	T	400	08T	C6-N6	2.57	1.42	1.34
2	W	400	08T	C6-N6	2.57	1.42	1.34
2	H	400	08T	C6-N6	2.58	1.42	1.34
2	P	400	08T	C6-N6	2.58	1.42	1.34
2	I	400	08T	C6-N6	2.59	1.42	1.34
2	E	400	08T	C6-N6	2.59	1.42	1.34
2	Q	400	08T	C6-N6	2.59	1.42	1.34
2	D	400	08T	C6-N6	2.60	1.43	1.34
2	B	400	08T	C6-N6	2.60	1.43	1.34
2	U	400	08T	C6-N6	2.61	1.43	1.34
2	V	400	08T	C6-N6	2.63	1.43	1.34
2	N	400	08T	C6-N6	2.63	1.43	1.34
4	X	400	ADP	C5-C4	2.98	1.47	1.40
4	L	400	ADP	C5-C4	3.01	1.47	1.40
2	D	400	08T	C2-N3	3.16	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	400	08T	C2-N3	3.22	1.37	1.32
2	O	400	08T	C2-N3	3.22	1.37	1.32
2	C	400	08T	C2-N3	3.24	1.37	1.32
2	M	400	08T	C2-N3	3.29	1.38	1.32
2	J	400	08T	C2-N3	3.29	1.38	1.32
2	S	400	08T	C2-N3	3.31	1.38	1.32
2	B	400	08T	C2-N3	3.31	1.38	1.32
2	K	400	08T	C2-N3	3.31	1.38	1.32
2	G	400	08T	C2-N3	3.32	1.38	1.32
2	V	400	08T	C2-N3	3.33	1.38	1.32
2	N	400	08T	C2-N3	3.33	1.38	1.32
2	T	400	08T	C2-N3	3.34	1.38	1.32
2	E	400	08T	C2-N3	3.35	1.38	1.32
2	W	400	08T	C2-N3	3.36	1.38	1.32
2	P	400	08T	C2-N3	3.37	1.38	1.32
2	Q	400	08T	C2-N3	3.39	1.38	1.32
2	U	400	08T	C2-N3	3.42	1.38	1.32
2	I	400	08T	C2-N3	3.42	1.38	1.32
2	H	400	08T	C2-N3	3.49	1.38	1.32
2	G	400	08T	O4'-C1'	6.68	1.49	1.41
2	J	400	08T	O4'-C1'	6.73	1.49	1.41
2	C	400	08T	O4'-C1'	6.82	1.49	1.41
2	M	400	08T	O4'-C1'	6.82	1.49	1.41
2	O	400	08T	O4'-C1'	6.82	1.49	1.41
2	V	400	08T	O4'-C1'	6.85	1.49	1.41
2	W	400	08T	O4'-C1'	6.92	1.49	1.41
2	I	400	08T	O4'-C1'	6.92	1.50	1.41
2	K	400	08T	O4'-C1'	6.94	1.50	1.41
2	U	400	08T	O4'-C1'	6.95	1.50	1.41
2	A	400	08T	O4'-C1'	6.96	1.50	1.41
2	B	400	08T	O4'-C1'	7.03	1.50	1.41
2	T	400	08T	O4'-C1'	7.05	1.50	1.41
2	D	400	08T	O4'-C1'	7.05	1.50	1.41
2	S	400	08T	O4'-C1'	7.06	1.50	1.41
2	Q	400	08T	O4'-C1'	7.07	1.50	1.41
2	E	400	08T	O4'-C1'	7.11	1.50	1.41
2	P	400	08T	O4'-C1'	7.15	1.50	1.41
2	N	400	08T	O4'-C1'	7.18	1.50	1.41
2	H	400	08T	O4'-C1'	7.25	1.50	1.41

All (187) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	400	08T	N3-C2-N1	-11.70	119.94	128.89
2	D	400	08T	N3-C2-N1	-11.69	119.95	128.89
2	A	400	08T	N3-C2-N1	-11.68	119.95	128.89
2	G	400	08T	N3-C2-N1	-11.66	119.96	128.89
2	H	400	08T	N3-C2-N1	-11.61	120.01	128.89
2	P	400	08T	N3-C2-N1	-11.60	120.01	128.89
2	J	400	08T	N3-C2-N1	-11.59	120.02	128.89
2	E	400	08T	N3-C2-N1	-11.57	120.03	128.89
2	S	400	08T	N3-C2-N1	-11.56	120.04	128.89
2	U	400	08T	N3-C2-N1	-11.53	120.06	128.89
2	M	400	08T	N3-C2-N1	-11.52	120.07	128.89
2	W	400	08T	N3-C2-N1	-11.51	120.08	128.89
2	C	400	08T	N3-C2-N1	-11.50	120.09	128.89
2	T	400	08T	N3-C2-N1	-11.50	120.09	128.89
2	K	400	08T	N3-C2-N1	-11.48	120.11	128.89
2	I	400	08T	N3-C2-N1	-11.46	120.12	128.89
2	V	400	08T	N3-C2-N1	-11.45	120.12	128.89
2	Q	400	08T	N3-C2-N1	-11.32	120.23	128.89
2	N	400	08T	N3-C2-N1	-11.31	120.23	128.89
2	O	400	08T	N3-C2-N1	-10.94	120.52	128.89
4	X	400	ADP	N3-C2-N1	-7.63	123.05	128.89
4	L	400	ADP	N3-C2-N1	-7.61	123.07	128.89
2	J	400	08T	C4'-O4'-C1'	-5.35	103.84	109.72
2	D	400	08T	C4'-O4'-C1'	-5.18	104.02	109.72
2	E	400	08T	C4'-O4'-C1'	-5.17	104.04	109.72
2	O	400	08T	C4'-O4'-C1'	-5.10	104.11	109.72
2	N	400	08T	C4'-O4'-C1'	-5.07	104.15	109.72
2	A	400	08T	PB-O3A-PA	-4.95	119.21	132.99
2	G	400	08T	C4'-O4'-C1'	-4.93	104.30	109.72
2	Q	400	08T	PB-O3A-PA	-4.86	119.47	132.99
2	I	400	08T	C4'-O4'-C1'	-4.81	104.44	109.72
2	P	400	08T	C4'-O4'-C1'	-4.58	104.69	109.72
2	C	400	08T	PB-O3A-PA	-4.56	120.30	132.99
2	S	400	08T	C4'-O4'-C1'	-4.50	104.78	109.72
2	B	400	08T	C4'-O4'-C1'	-4.48	104.80	109.72
2	E	400	08T	PB-O3A-PA	-4.47	120.55	132.99
2	V	400	08T	C4'-O4'-C1'	-4.45	104.83	109.72
2	A	400	08T	C4'-O4'-C1'	-4.40	104.88	109.72
2	M	400	08T	PB-O3A-PA	-4.38	120.78	132.99
2	I	400	08T	PB-O3A-PA	-4.26	121.13	132.99
2	U	400	08T	C4'-O4'-C1'	-4.24	105.06	109.72
2	W	400	08T	C4'-O4'-C1'	-4.24	105.06	109.72
2	U	400	08T	PB-O3A-PA	-4.22	121.24	132.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	400	08T	C4'-O4'-C1'	-4.20	105.11	109.72
2	Q	400	08T	C4'-O4'-C1'	-4.19	105.11	109.72
2	K	400	08T	C4'-O4'-C1'	-4.16	105.15	109.72
2	J	400	08T	O2B-PB-O1B	-4.15	106.34	118.70
2	S	400	08T	PB-O3A-PA	-4.10	121.57	132.99
2	N	400	08T	C2'-C1'-N9	-4.04	108.12	114.29
2	T	400	08T	C4'-O4'-C1'	-4.03	105.29	109.72
2	N	400	08T	PB-O3A-PA	-3.99	121.86	132.99
2	M	400	08T	C4'-O4'-C1'	-3.95	105.38	109.72
2	O	400	08T	C2'-C1'-N9	-3.93	108.28	114.29
2	H	400	08T	C4'-O4'-C1'	-3.89	105.44	109.72
2	W	400	08T	PB-O3A-PA	-3.83	122.32	132.99
2	H	400	08T	PB-O3A-PA	-3.83	122.33	132.99
2	O	400	08T	PB-O3A-PA	-3.80	122.41	132.99
2	K	400	08T	PB-O3A-PA	-3.79	122.42	132.99
2	D	400	08T	PB-O3A-PA	-3.68	122.75	132.99
2	G	400	08T	O2B-PB-O1B	-3.68	107.75	118.70
2	P	400	08T	PB-O3A-PA	-3.65	122.83	132.99
2	K	400	08T	O1A-PA-O2A	-3.53	108.18	118.70
2	W	400	08T	O1A-PA-O2A	-3.52	108.21	118.70
2	J	400	08T	C2'-C1'-N9	-3.47	108.99	114.29
2	S	400	08T	O2B-PB-O1B	-3.44	108.44	118.70
2	E	400	08T	O1A-PA-O2A	-3.44	108.44	118.70
2	D	400	08T	C2'-C1'-N9	-3.42	109.06	114.29
2	H	400	08T	O1A-PA-O2A	-3.42	108.51	118.70
2	N	400	08T	O1A-PA-O2A	-3.42	108.52	118.70
2	G	400	08T	C2'-C1'-N9	-3.42	109.07	114.29
2	E	400	08T	C2'-C1'-N9	-3.39	109.11	114.29
2	S	400	08T	O1A-PA-O2A	-3.38	108.63	118.70
2	P	400	08T	O1A-PA-O2A	-3.38	108.63	118.70
2	T	400	08T	O1A-PA-O2A	-3.38	108.64	118.70
2	K	400	08T	C2'-C1'-N9	-3.37	109.14	114.29
2	B	400	08T	O1A-PA-O2A	-3.35	108.71	118.70
4	L	400	ADP	C4-C5-N7	-3.31	106.44	109.48
2	B	400	08T	PB-O3A-PA	-3.30	123.79	132.99
2	V	400	08T	O1A-PA-O2A	-3.30	108.86	118.70
4	X	400	ADP	PA-O3A-PB	-3.28	121.68	132.67
2	U	400	08T	O1A-PA-O2A	-3.21	109.12	118.70
2	V	400	08T	PB-O3A-PA	-3.21	124.04	132.99
2	I	400	08T	O1A-PA-O2A	-3.21	109.14	118.70
2	A	400	08T	C2'-C1'-N9	-3.18	109.44	114.29
2	C	400	08T	O1A-PA-O2A	-3.18	109.24	118.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	400	08T	O1A-PA-O2A	-3.17	109.26	118.70
2	C	400	08T	C2'-C1'-N9	-3.16	109.46	114.29
2	D	400	08T	O1A-PA-O2A	-3.16	109.30	118.70
2	A	400	08T	O2B-PB-O1B	-3.13	109.38	118.70
4	X	400	ADP	C4-C5-N7	-3.09	106.64	109.48
2	M	400	08T	O2B-PB-O1B	-3.08	109.51	118.70
2	S	400	08T	C2'-C1'-N9	-3.08	109.59	114.29
2	B	400	08T	C2'-C1'-N9	-3.06	109.62	114.29
2	E	400	08T	O2B-PB-O1B	-3.06	109.60	118.70
2	O	400	08T	O1A-PA-O2A	-3.04	109.64	118.70
2	P	400	08T	C2'-C1'-N9	-3.03	109.66	114.29
2	M	400	08T	O1A-PA-O2A	-3.03	109.68	118.70
2	H	400	08T	O2B-PB-O1B	-3.01	109.74	118.70
2	Q	400	08T	O2B-PB-O1B	-3.00	109.75	118.70
2	G	400	08T	PB-O3A-PA	-2.98	124.69	132.99
2	A	400	08T	O1A-PA-O2A	-2.96	109.89	118.70
2	W	400	08T	C2'-C1'-N9	-2.92	109.82	114.29
2	V	400	08T	C2'-C1'-N9	-2.92	109.82	114.29
2	J	400	08T	O1A-PA-O2A	-2.89	110.09	118.70
2	N	400	08T	O2B-PB-O1B	-2.88	110.11	118.70
2	U	400	08T	O2B-PB-O1B	-2.88	110.11	118.70
2	G	400	08T	O1A-PA-O2A	-2.86	110.18	118.70
2	M	400	08T	C2'-C1'-N9	-2.85	109.94	114.29
2	D	400	08T	O2B-PB-O1B	-2.81	110.33	118.70
2	I	400	08T	O2B-PB-O1B	-2.75	110.52	118.70
2	P	400	08T	O2B-PB-O1B	-2.74	110.53	118.70
2	C	400	08T	O2B-PB-O1B	-2.70	110.66	118.70
2	K	400	08T	O2B-PB-O1B	-2.68	110.70	118.70
2	B	400	08T	O2B-PB-O1B	-2.67	110.75	118.70
2	O	400	08T	O2B-PB-O1B	-2.66	110.77	118.70
2	J	400	08T	PB-O3A-PA	-2.66	125.58	132.99
2	T	400	08T	O2B-PB-O1B	-2.66	110.78	118.70
2	U	400	08T	C2'-C1'-N9	-2.62	110.29	114.29
2	T	400	08T	PB-O3A-PA	-2.61	125.72	132.99
2	W	400	08T	O2B-PB-O1B	-2.60	110.95	118.70
4	L	400	ADP	PA-O3A-PB	-2.56	124.07	132.67
2	V	400	08T	O2B-PB-O1B	-2.55	111.11	118.70
2	Q	400	08T	C2'-C1'-N9	-2.46	110.53	114.29
2	I	400	08T	C2'-C1'-N9	-2.45	110.54	114.29
2	T	400	08T	C2'-C1'-N9	-2.39	110.64	114.29
2	H	400	08T	C2'-C1'-N9	-2.36	110.68	114.29
4	L	400	ADP	C2'-C1'-N9	-2.35	110.70	114.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	X	400	ADP	C2'-C1'-N9	-2.06	111.14	114.29
2	O	400	08T	C1'-N9-C4	2.02	129.99	126.94
2	Q	400	08T	C1'-N9-C4	2.05	130.03	126.94
2	J	400	08T	C2'-C3'-C4'	2.06	106.84	102.61
2	T	400	08T	C1'-N9-C4	2.13	130.15	126.94
2	W	400	08T	O3A-PA-O5'	2.16	109.66	101.36
2	K	400	08T	O3A-PA-O5'	2.21	109.87	101.36
2	I	400	08T	O3A-PB-O3B	2.22	109.76	101.31
2	B	400	08T	O3A-PB-O3B	2.23	109.81	101.31
2	Q	400	08T	C2'-C3'-C4'	2.24	107.22	102.61
2	P	400	08T	O3A-PA-O5'	2.33	110.32	101.36
2	J	400	08T	O3A-PB-O3B	2.34	110.22	101.31
2	T	400	08T	O3A-PA-O5'	2.37	110.46	101.36
2	H	400	08T	C1'-N9-C4	2.40	130.57	126.94
2	E	400	08T	O3A-PA-O5'	2.41	110.61	101.36
2	G	400	08T	C2'-C3'-C4'	2.42	107.59	102.61
2	S	400	08T	O3A-PA-O5'	2.43	110.70	101.36
2	S	400	08T	O3A-PB-O3B	2.49	110.79	101.31
2	U	400	08T	O3A-PB-O3B	2.52	110.90	101.31
2	A	400	08T	O3A-PB-O3B	2.54	110.96	101.31
2	O	400	08T	O3A-PB-O3B	2.61	111.25	101.31
2	M	400	08T	O3A-PA-O5'	2.68	111.66	101.36
2	N	400	08T	O3A-PA-O5'	2.68	111.66	101.36
2	W	400	08T	O3A-PB-O3B	2.68	111.51	101.31
2	M	400	08T	O3A-PB-O3B	2.72	111.66	101.31
2	K	400	08T	O3A-PB-O3B	2.74	111.72	101.31
2	C	400	08T	O3A-PB-O3B	2.78	111.87	101.31
2	T	400	08T	O3A-PB-O3B	2.79	111.91	101.31
2	H	400	08T	O3A-PA-O5'	2.84	112.28	101.36
2	Q	400	08T	O3A-PB-O3B	2.87	112.22	101.31
2	J	400	08T	O3A-PA-O5'	2.93	112.62	101.36
2	Q	400	08T	O3A-PA-O5'	2.96	112.74	101.36
2	D	400	08T	O3A-PB-O3B	2.97	112.62	101.31
2	O	400	08T	O3A-PA-O5'	3.03	113.01	101.36
2	E	400	08T	O3A-PB-O3B	3.05	112.90	101.31
2	N	400	08T	O3A-PB-O3B	3.06	112.97	101.31
2	G	400	08T	O3A-PB-O3B	3.16	113.34	101.31
2	A	400	08T	O3A-PA-O5'	3.38	114.37	101.36
2	H	400	08T	O3A-PB-O3B	3.51	114.67	101.31
2	N	400	08T	C1'-N9-C4	3.52	132.26	126.94
2	J	400	08T	C4-C5-N7	5.85	114.86	109.48
2	E	400	08T	C4-C5-N7	5.93	114.94	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	400	08T	C4-C5-N7	5.94	114.94	109.48
2	D	400	08T	C4-C5-N7	5.99	114.99	109.48
2	T	400	08T	C4-C5-N7	6.08	115.07	109.48
2	A	400	08T	C4-C5-N7	6.08	115.07	109.48
2	S	400	08T	C4-C5-N7	6.10	115.09	109.48
2	G	400	08T	C4-C5-N7	6.10	115.09	109.48
2	V	400	08T	C4-C5-N7	6.11	115.10	109.48
2	C	400	08T	C4-C5-N7	6.12	115.11	109.48
2	U	400	08T	C4-C5-N7	6.12	115.11	109.48
2	P	400	08T	C4-C5-N7	6.12	115.11	109.48
2	I	400	08T	C4-C5-N7	6.12	115.11	109.48
2	B	400	08T	C4-C5-N7	6.12	115.11	109.48
2	M	400	08T	C4-C5-N7	6.14	115.12	109.48
2	O	400	08T	C4-C5-N7	6.14	115.13	109.48
2	H	400	08T	C4-C5-N7	6.17	115.16	109.48
2	K	400	08T	C4-C5-N7	6.18	115.16	109.48
2	N	400	08T	C4-C5-N7	6.27	115.25	109.48
2	W	400	08T	C4-C5-N7	6.34	115.31	109.48

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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	247/268 (92%)	-0.10	2 (0%) 87 78	141, 179, 214, 236	0
1	B	247/268 (92%)	-0.01	4 (1%) 74 61	87, 146, 181, 196	0
1	C	247/268 (92%)	-0.05	2 (0%) 87 78	90, 138, 183, 202	0
1	D	247/268 (92%)	-0.08	0 100 100	78, 122, 152, 179	0
1	E	247/268 (92%)	-0.01	0 100 100	80, 123, 154, 195	0
1	F	247/268 (92%)	-0.07	3 (1%) 81 69	91, 154, 216, 241	0
1	G	247/268 (92%)	0.34	24 (9%) 10 7	156, 188, 226, 240	0
1	H	247/268 (92%)	-0.05	0 100 100	89, 144, 180, 196	0
1	I	247/268 (92%)	-0.04	1 (0%) 93 88	92, 129, 184, 211	0
1	J	247/268 (92%)	0.00	2 (0%) 87 78	88, 128, 160, 180	0
1	K	247/268 (92%)	0.04	0 100 100	87, 125, 159, 189	0
1	L	247/268 (92%)	0.19	15 (6%) 25 16	95, 165, 254, 273	0
1	M	247/268 (92%)	-0.01	4 (1%) 74 61	128, 173, 203, 219	0
1	N	247/268 (92%)	-0.02	2 (0%) 87 78	87, 141, 177, 209	0
1	O	247/268 (92%)	-0.07	0 100 100	89, 134, 184, 220	0
1	P	247/268 (92%)	-0.03	0 100 100	83, 126, 157, 186	0
1	Q	247/268 (92%)	0.02	1 (0%) 93 88	74, 124, 154, 195	0
1	R	247/268 (92%)	0.02	5 (2%) 68 54	97, 161, 224, 242	0
1	S	247/268 (92%)	0.30	21 (8%) 13 10	155, 190, 226, 239	0
1	T	247/268 (92%)	-0.05	0 100 100	95, 146, 181, 199	0
1	U	247/268 (92%)	-0.04	1 (0%) 93 88	86, 135, 187, 210	0
1	V	247/268 (92%)	-0.05	2 (0%) 87 78	82, 126, 158, 200	0
1	W	247/268 (92%)	-0.08	1 (0%) 93 88	83, 125, 161, 192	0
1	X	247/268 (92%)	0.19	14 (5%) 27 19	102, 165, 252, 273	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
All	All	5928/6432 (92%)	0.01	104 (1%)	71	58	74, 143, 210, 273	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	363	ILE	7.5
1	X	363	ILE	7.2
1	L	344	GLN	7.0
1	X	344	GLN	6.9
1	G	215	ALA	5.6
1	X	333	ALA	5.0
1	S	297	TYR	5.0
1	G	277	ALA	4.7
1	S	149	ILE	4.7
1	X	361	ASN	4.6
1	L	361	ASN	4.4
1	L	141	PHE	4.1
1	X	331	LYS	4.0
1	G	237	LEU	4.0
1	G	149	ILE	4.0
1	G	221	SER	3.9
1	L	345	GLU	3.8
1	R	300	LEU	3.8
1	G	240	ILE	3.7
1	G	271	VAL	3.6
1	S	303	ILE	3.6
1	G	292	PHE	3.4
1	G	220	VAL	3.4
1	X	320	LEU	3.3
1	S	206	ALA	3.3
1	G	223	LYS	3.2
1	R	139	TYR	3.1
1	L	339	PHE	3.1
1	L	139	TYR	3.1
1	B	160	GLU	3.1
1	B	382	CYS	3.1
1	F	322	ASN	3.1
1	S	196	VAL	3.1
1	G	165	ILE	3.1
1	N	337	GLU	3.0
1	U	139	TYR	3.0
1	G	188	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	S	164	LEU	3.0
1	S	292	PHE	3.0
1	X	382	CYS	2.9
1	L	378	GLY	2.9
1	G	194	LEU	2.9
1	G	246	GLU	2.9
1	G	196	VAL	2.8
1	R	322	ASN	2.8
1	V	301	GLY	2.8
1	S	177	ALA	2.8
1	S	220	VAL	2.8
1	S	215	ALA	2.7
1	S	246	GLU	2.7
1	X	345	GLU	2.7
1	L	320	LEU	2.7
1	G	266	ARG	2.7
1	W	158	CYS	2.6
1	N	301	GLY	2.6
1	A	153	ILE	2.6
1	X	139	TYR	2.6
1	G	301	GLY	2.6
1	R	361	ASN	2.6
1	C	300	LEU	2.5
1	F	139	TYR	2.5
1	S	237	LEU	2.4
1	G	373	LYS	2.4
1	S	304	GLU	2.4
1	L	347	LEU	2.4
1	S	296	LEU	2.4
1	L	341	LYS	2.4
1	G	164	LEU	2.4
1	M	305	ILE	2.4
1	J	301	GLY	2.4
1	G	365	ARG	2.3
1	S	195	ASN	2.3
1	F	332	TYR	2.3
1	L	333	ALA	2.3
1	Q	265	GLY	2.3
1	L	380	LEU	2.3
1	B	141	PHE	2.3
1	J	374	PHE	2.3
1	M	218	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	S	255	ILE	2.2
1	X	367	VAL	2.2
1	B	347	LEU	2.2
1	X	215	ALA	2.2
1	C	196	VAL	2.2
1	A	292	PHE	2.2
1	L	362	VAL	2.2
1	S	382	CYS	2.2
1	M	277	ALA	2.2
1	L	346	LEU	2.2
1	S	347	LEU	2.2
1	X	275	ILE	2.2
1	X	348	LEU	2.2
1	R	138	GLU	2.1
1	M	215	ALA	2.1
1	S	277	ALA	2.1
1	S	306	GLU	2.1
1	G	278	ALA	2.1
1	X	371	GLU	2.1
1	S	310	LEU	2.0
1	G	293	ARG	2.0
1	G	216	PHE	2.0
1	V	220	VAL	2.0
1	G	316	ASP	2.0
1	I	243	LEU	2.0

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, 95th percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	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	0.14	79,125,156,158	42
2	08T	N	400	31/31	0.91	0.28	0.08	95,118,141,155	42
3	MG	C	401	1/1	0.96	0.27	0.03	82,82,82,82	0
3	MG	V	401	1/1	0.92	0.27	0.02	113,113,113,113	0
3	MG	T	401	1/1	0.95	0.24	0.02	129,129,129,129	0
2	08T	P	400	31/31	0.94	0.29	0.02	80,102,124,131	42
2	08T	E	400	31/31	0.92	0.27	-0.00	86,115,137,160	42
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
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	-0.05	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	0.88	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
3	MG	A	401	1/1	0.97	0.18	-0.54	140,140,140,140	1
2	08T	G	400	31/31	0.89	0.24	-0.54	117,149,177,182	42
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	-1.28	118,118,118,118	1
3	MG	M	401	1/1	0.96	0.15	-1.30	133,133,133,133	1
3	MG	P	401	1/1	0.75	0.21	-1.49	113,113,113,113	0
3	MG	B	401	1/1	0.88	0.17	-1.80	112,112,112,112	0
3	MG	Q	401	1/1	0.66	0.22	-1.82	125,125,125,125	1
3	MG	N	401	1/1	0.87	0.14	-1.99	96,96,96,96	1
3	MG	E	401	1/1	0.89	0.16	-2.50	95,95,95,95	0
3	MG	W	401	1/1	0.92	0.13	-2.93	109,109,109,109	0
3	MG	D	401	1/1	0.90	0.12	-2.96	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	-3.79	111,111,111,111	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
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.