



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 27, 2016 – 11:41 AM EDT

PDB ID : 5D4D  
Title : Crystal structure of Thermus thermophilus product complex for transcription initiation with NAD and CTP  
Authors : Zhang, Y.; Ebright, R.H.  
Deposited on : 2015-08-07  
Resolution : 3.00 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](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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027939  
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) : rb-20027939

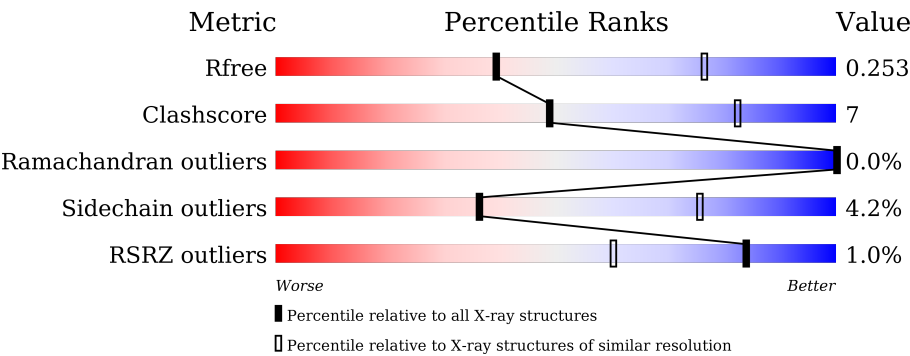
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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.









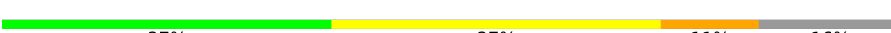



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	315	<div><div></div><div>56%17%27%</div></div>
1	B	315	<div><div></div><div>56%14%30%</div></div>
1	K	315	<div><div></div><div>54%18%28%</div></div>
1	L	315	<div><div></div><div>52%17%30%</div></div>
2	C	1119	<div><div>%</div><div>80%18%..</div></div>
2	M	1119	<div><div>3%</div><div>72%24%..</div></div>

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Mol	Chain	Length	Quality of chain
3	D	1524	
3	N	1524	
4	E	99	
4	O	99	
5	F	443	
5	P	443	
6	G	19	
6	R	19	
7	H	27	
7	S	27	

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
13	A	R	101	-	-	-	X

## 2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 57349 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	229	Total	C	N	O	S	0	0	0
			1797	1147	313	335	2			
1	B	222	Total	C	N	O	S	0	0	0
			1750	1120	303	325	2			
1	K	228	Total	C	N	O	S	0	0	0
			1792	1144	312	334	2			
1	L	222	Total	C	N	O	S	0	0	0
			1750	1120	303	325	2			

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1108	Total	C	N	O	S	0	0	0
			8747	5536	1561	1626	24			
2	M	1091	Total	C	N	O	S	0	0	0
			8611	5449	1539	1600	23			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1485	Total	C	N	O	S	0	0	0
			11730	7435	2066	2194	35			
3	N	1483	Total	C	N	O	S	0	0	0
			11716	7427	2064	2190	35			

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	94	Total	C	N	O	S	0	0	0
			758	483	132	139	4			
4	O	94	Total	C	N	O	S	0	0	0
			758	483	132	139	4			

- Molecule 5 is a protein called RNA polymerase sigma factor SigA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	346	Total	C	N	O	S	0	0	0
			2807	1770	509	524	4			
5	P	316	Total	C	N	O	S	0	0	0
			2574	1624	466	480	4			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-19	MET	-	initiating methionine	UNP Q72L95
F	-18	GLY	-	expression tag	UNP Q72L95
F	-17	SER	-	expression tag	UNP Q72L95
F	-16	SER	-	expression tag	UNP Q72L95
F	-15	HIS	-	expression tag	UNP Q72L95
F	-14	HIS	-	expression tag	UNP Q72L95
F	-13	HIS	-	expression tag	UNP Q72L95
F	-12	HIS	-	expression tag	UNP Q72L95
F	-11	HIS	-	expression tag	UNP Q72L95
F	-10	HIS	-	expression tag	UNP Q72L95
F	-9	SER	-	expression tag	UNP Q72L95
F	-8	SER	-	expression tag	UNP Q72L95
F	-7	GLY	-	expression tag	UNP Q72L95
F	-6	LEU	-	expression tag	UNP Q72L95
F	-5	VAL	-	expression tag	UNP Q72L95
F	-4	PRO	-	expression tag	UNP Q72L95
F	-3	ARG	-	expression tag	UNP Q72L95
F	-2	GLY	-	expression tag	UNP Q72L95
F	-1	SER	-	expression tag	UNP Q72L95
F	0	HIS	-	expression tag	UNP Q72L95
F	46	THR	ALA	conflict	UNP Q72L95
P	-19	MET	-	initiating methionine	UNP Q72L95
P	-18	GLY	-	expression tag	UNP Q72L95
P	-17	SER	-	expression tag	UNP Q72L95
P	-16	SER	-	expression tag	UNP Q72L95
P	-15	HIS	-	expression tag	UNP Q72L95
P	-14	HIS	-	expression tag	UNP Q72L95
P	-13	HIS	-	expression tag	UNP Q72L95
P	-12	HIS	-	expression tag	UNP Q72L95
P	-11	HIS	-	expression tag	UNP Q72L95
P	-10	HIS	-	expression tag	UNP Q72L95
P	-9	SER	-	expression tag	UNP Q72L95
P	-8	SER	-	expression tag	UNP Q72L95
P	-7	GLY	-	expression tag	UNP Q72L95

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Chain	Residue	Modelled	Actual	Comment	Reference
P	-6	LEU	-	expression tag	UNP Q72L95
P	-5	VAL	-	expression tag	UNP Q72L95
P	-4	PRO	-	expression tag	UNP Q72L95
P	-3	ARG	-	expression tag	UNP Q72L95
P	-2	GLY	-	expression tag	UNP Q72L95
P	-1	SER	-	expression tag	UNP Q72L95
P	0	HIS	-	expression tag	UNP Q72L95
P	46	THR	ALA	conflict	UNP Q72L95

- Molecule 6 is a DNA chain called DNA (5'-D(\*CP\*C\*TP\*GP\*CP\*AP\*TP\*CP\*CP\*GP\*T  
P\*GP\*AP\*GP\*TP\*AP\*GP\*AP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	16	Total	C	N	O	P	0	0	0
			328	157	62	94	15			
6	R	16	Total	C	N	O	P	0	0	0
			328	157	62	94	15			

- Molecule 7 is a DNA chain called DNA (27-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	21	Total	C	N	O	P	0	0	0
			435	207	87	121	20			
7	S	21	Total	C	N	O	P	0	0	0
			434	206	87	121	20			

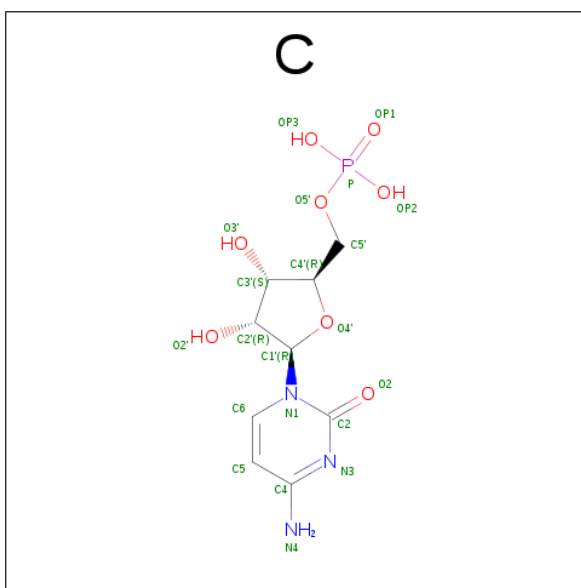
- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	P	1	Total	Mg	0	0
			1	1		
8	D	3	Total	Mg	0	0
			3	3		
8	B	1	Total	Mg	0	0
			1	1		
8	N	3	Total	Mg	0	0
			3	3		
8	L	1	Total	Mg	0	0
			1	1		
8	F	1	Total	Mg	0	0
			1	1		

- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

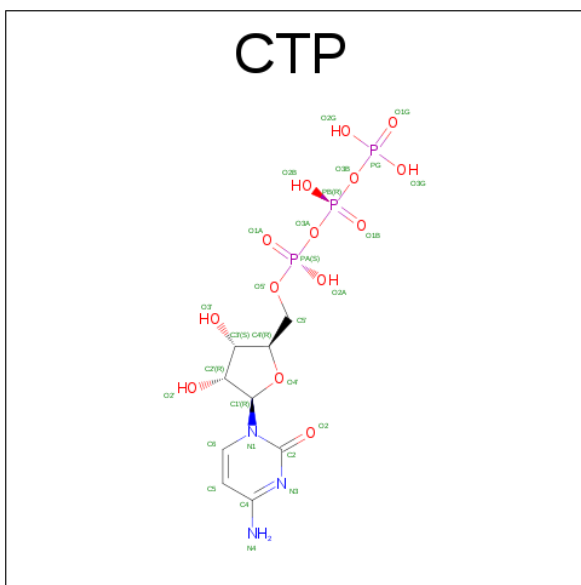
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	D	2	Total	Zn	0	0
			2	2		
9	N	2	Total	Zn	0	0
			2	2		

- Molecule 10 is CYTIDINE-5'-MONOPHOSPHATE (three-letter code: C) (formula: C<sub>9</sub>H<sub>14</sub>N<sub>3</sub>O<sub>8</sub>P).



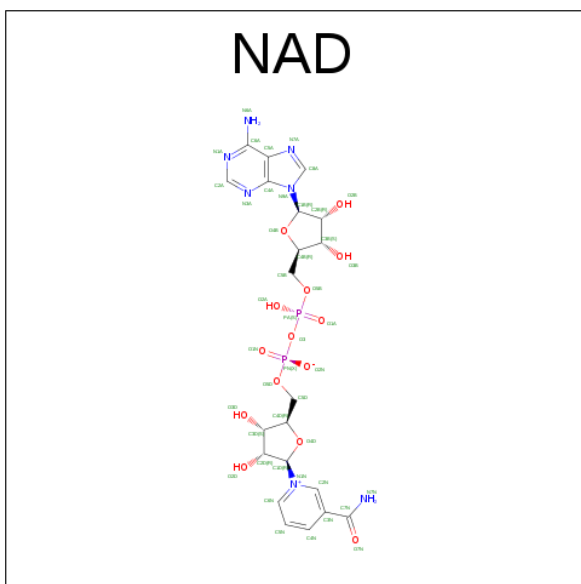
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	D	1	Total	C	N	O	P	0	0
			20	9	3	7	1		
10	N	1	Total	C	N	O	P	0	0
			20	9	3	7	1		

- Molecule 11 is CYTIDINE-5'-TRIPHOSPHATE (three-letter code: CTP) (formula: C<sub>9</sub>H<sub>16</sub>N<sub>3</sub>O<sub>14</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	D	1	Total 9	O 7	P 2	0	0
11	M	1	Total 9	O 7	P 2	0	0

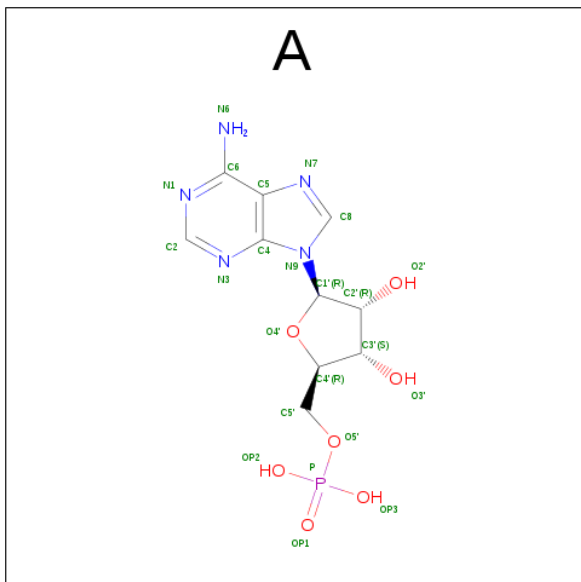
- Molecule 12 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula:  $C_{21}H_{27}N_7O_{14}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		



- Molecule 13 is ADENOSINE-5'-MONOPHOSPHATE (three-letter code: A) (formula:  $C_{10}H_{14}N_5O_7P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	R	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	23	Total	O	0	0
			23	23		
14	B	16	Total	O	0	0
			16	16		
14	C	196	Total	O	0	0
			196	196		
14	D	244	Total	O	0	0
			244	244		
14	E	16	Total	O	0	0
			16	16		
14	F	45	Total	O	0	0
			45	45		
14	G	8	Total	O	0	0
			8	8		
14	H	4	Total	O	0	0
			4	4		
14	K	14	Total	O	0	0
			14	14		

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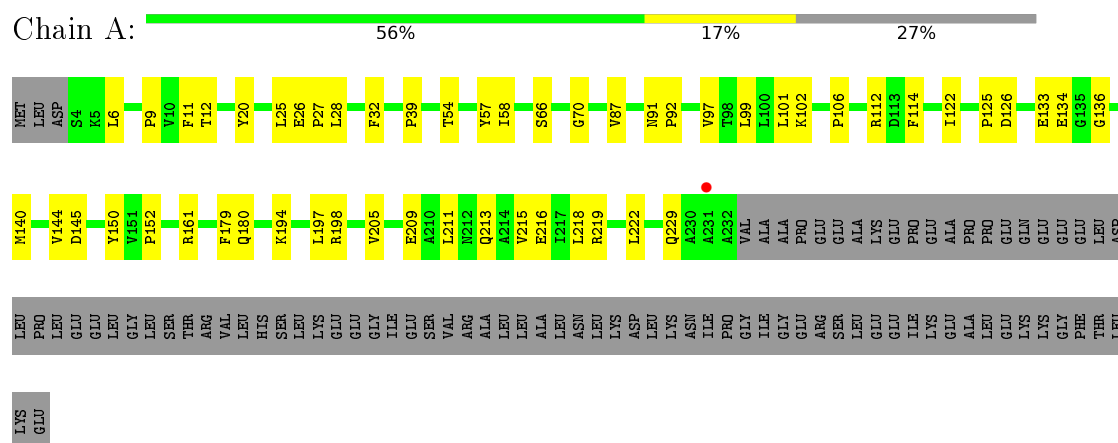
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	L	13	Total 13	O 13	0	0
14	M	97	Total 97	O 97	0	0
14	N	187	Total 187	O 187	0	0
14	O	12	Total 12	O 12	0	0
14	P	14	Total 14	O 14	0	0
14	R	3	Total 3	O 3	0	0
14	S	3	Total 3	O 3	0	0

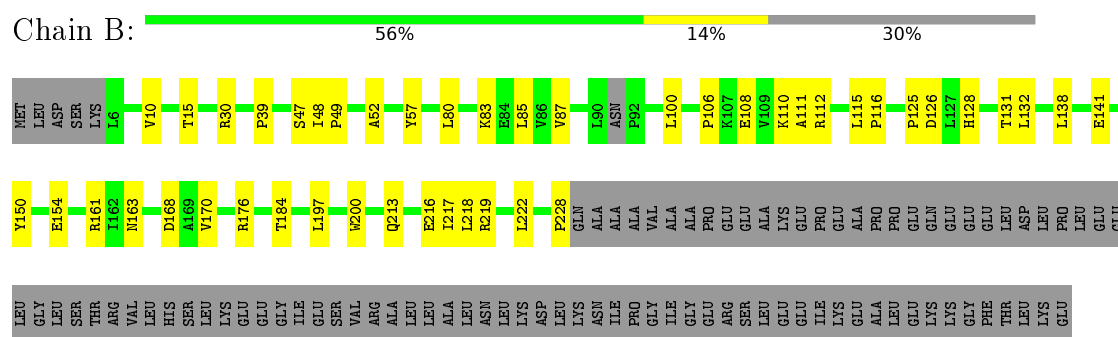
### 3 Residue-property plots

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.

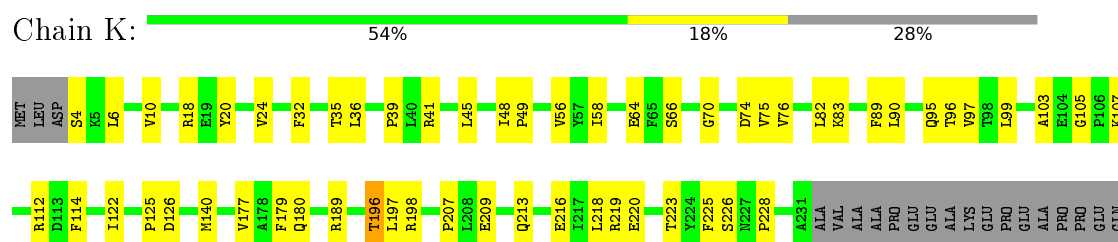
#### • Molecule 1: DNA-directed RNA polymerase subunit alpha



#### • Molecule 1: DNA-directed RNA polymerase subunit alpha



#### • Molecule 1: DNA-directed RNA polymerase subunit alpha



GLU  
GLU  
GLU  
LEU  
ASP  
LEU  
PRO  
LEU  
GLU  
GLU  
LEU  
LEU  
GLY  
LEU  
SER  
THR  
ARG  
VAL  
LEU  
HIS  
SER  
LEU  
GLU  
GLU  
GLY  
ILE  
GLU  
SER  
VAL  
ARG  
ALA  
LEU  
LEU  
ALA  
LEU  
ASN  
LEU  
LYS  
ASP  
LEU  
LYS  
ASN  
ILE  
PRO  
GLY  
ILE  
GLY  
GLU  
ARG  
SER  
LEU  
GLU  
GLU  
ILE  
LYS  
GLU  
ALA  
LEU  
GLU  
LYS

LYS  
GLY  
PHE  
THR  
LEU  
LYS  
GLU

• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain L:  52% 17% 30%


MET  
LEU  
ASP  
SER  
L6  
L36  
P39  
L30  
R41  
V56  
Y57  
E64  
T67  
V71  
K72  
E73  
D74  
E77  
I78  
I79  
L80  
N81  
L82  
K83  
L90  
ASN  
P92  
S93  
L94  
Q95  
T96  
V97  
L101  
E108  
V109  
K110  
A111  
R112  
D113  
F114  
P116  
P125  
D126  
L127  
H128  
T131

L132  
L138  
V142  
R143  
V144  
D145  
D146  
Y150  
A153  
E154  
H156  
G157  
I158  
R161  
I162  
N163  
A164  
I165  
D168  
A169  
V170  
R175  
R176  
V177  
A178  
F179  
R185  
L186  
G187  
L197  
W200  
E220  
H221  
L222  
T223  
P228  
G1N  
ALA  
ALA  
VAL  
ALA  
ALA  
PRO  
GLU  
GLU  
ALA

LYS  
GLU  
PRO  
GLY  
ALA  
PRO  
PRO  
GLU  
GLU  
GLU  
GLU  
GLY  
LEU  
ASP  
LEU  
PRO  
GLU  
GLU  
GLY  
PHE  
THR  
LEU  
LYS  
GLU

GLU  
GLU  
ILE  
LYS  
GLU  
ALA  
LEU  
GLU  
LYS  
LYS  
PHE  
THR  
LEU  
LYS  
GLU

• Molecule 2: DNA-directed RNA polymerase subunit beta

Chain C:  80% 18% 2%

H1  
R5  
V12  
I13  
R28  
D33  
V34  
P35  
P36  
E37  
K38  
N41  
V42  
O43  
A46  
E56  
GLU  
ASP  
LYS  
LYS  
GLY  
G63  
L64  
E70  
G74  
E75  
P76  
P77  
D87  
A92  
P93  
R97  
L100  
K103  
D104  
T105  
G106  
E110  
I118  
P119  
L120  
D133

R134  
H141  
V146  
A160  
S161  
I162  
L165  
R168  
I172  
D173  
L174  
G175  
V176  
E177  
P178  
V182  
S183  
M184  
R185  
M359  
L360  
M361  
V199  
L200  
E205  
T206  
R209  
E210  
L211  
G212  
L217  
V218  
Q219  
M222  
E224  
S225  
M229  
E232  
E233  
D246  
R250  
T261

Y267  
D268  
K280  
R284  
L285  
D300  
Y309  
D324  
H327  
L328  
G329  
N330  
Q343  
F344  
L351  
R358  
M359  
L360  
M361  
GLY  
SER  
GLU  
ASP  
S366  
L367  
L372  
S375  
A380  
E384  
F385  
S392  
K395  
D396  
E397  
R405  
R409  
L413  
R420  
E421  
T261

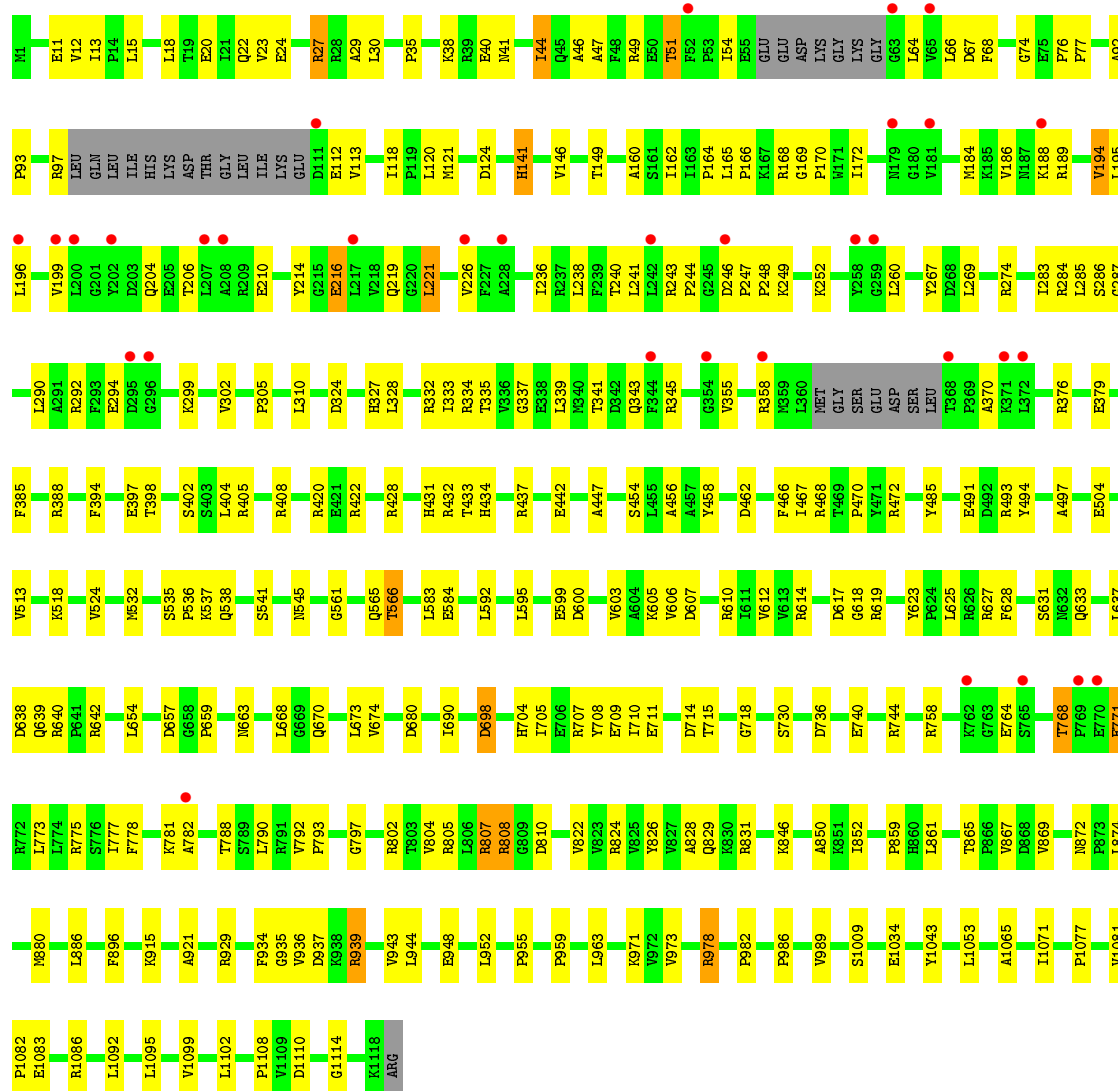
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D429  
Q436  
A447  
I452  
T453  
S454  
D462  
R468  
R472  
V483  
T489  
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V524  
Q538  
M545  
T566  
Q575  
L583  
L595  
V596  
A597  
E598  
E599  
D600  
K605  
V606  
D607  
R610  
I611  
V612  
D617  
S618  
R619  
R626  
R627  
F628  
R629  
G630  
S631

R632  
Q633  
L637  
D638  
R642  
V645  
L655  
A656  
Q670  
V674  
R674  
F684  
I690  
E693  
K696  
F699  
Y708  
E711  
L717  
P727  
D738  
G757  
G763  
E766  
P767  
T768  
E771  
R783  
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L790  
R791  
V792  
P793  
G797  
R805

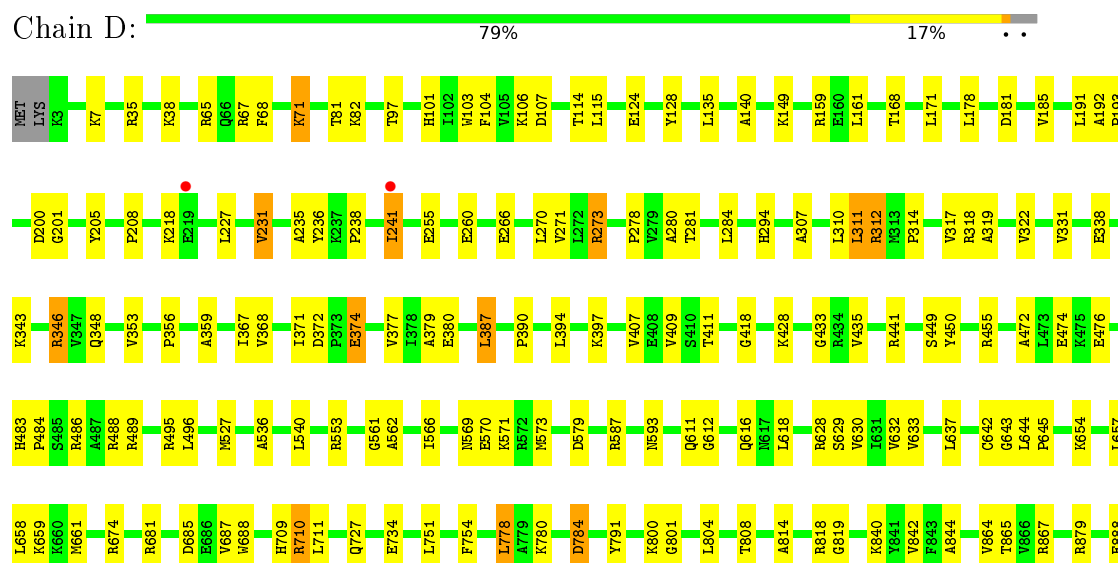
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R807  
D810  
L815  
K816  
Y819  
V822  
Q829  
P854  
V855  
P862  
V869  
R872  
L874  
R881  
Q884  
T888  
I902  
E916  
Q920  
F921  
F922  
R930  
F934  
G935  
V936  
D937  
R938  
R939  
L944  
R945  
R946  
L952  
P959  
K964  
Y975  
D976

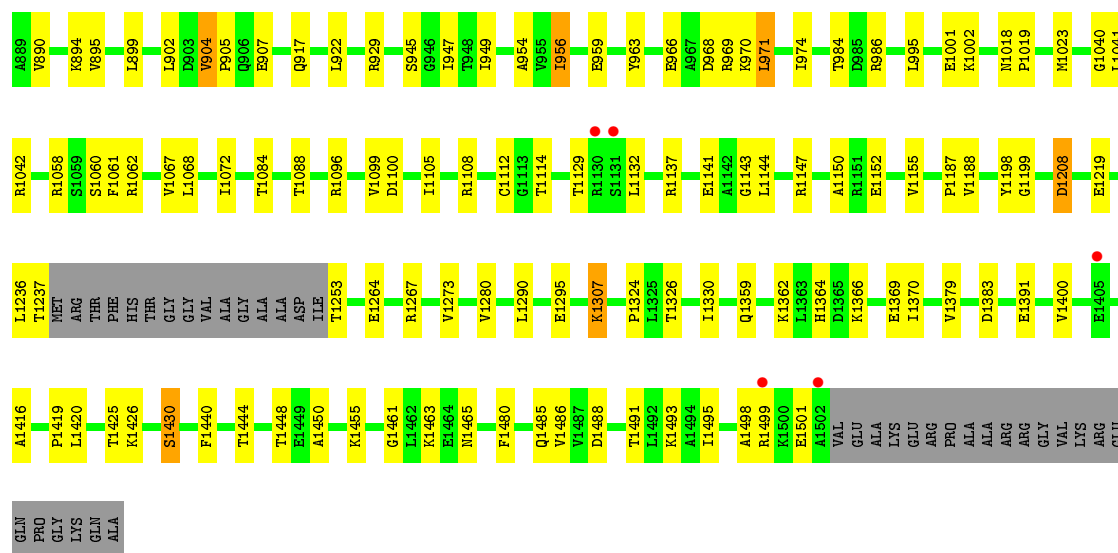
• Molecule 2: DNA-directed RNA polymerase subunit beta

Chain M:  72% 24% 3%

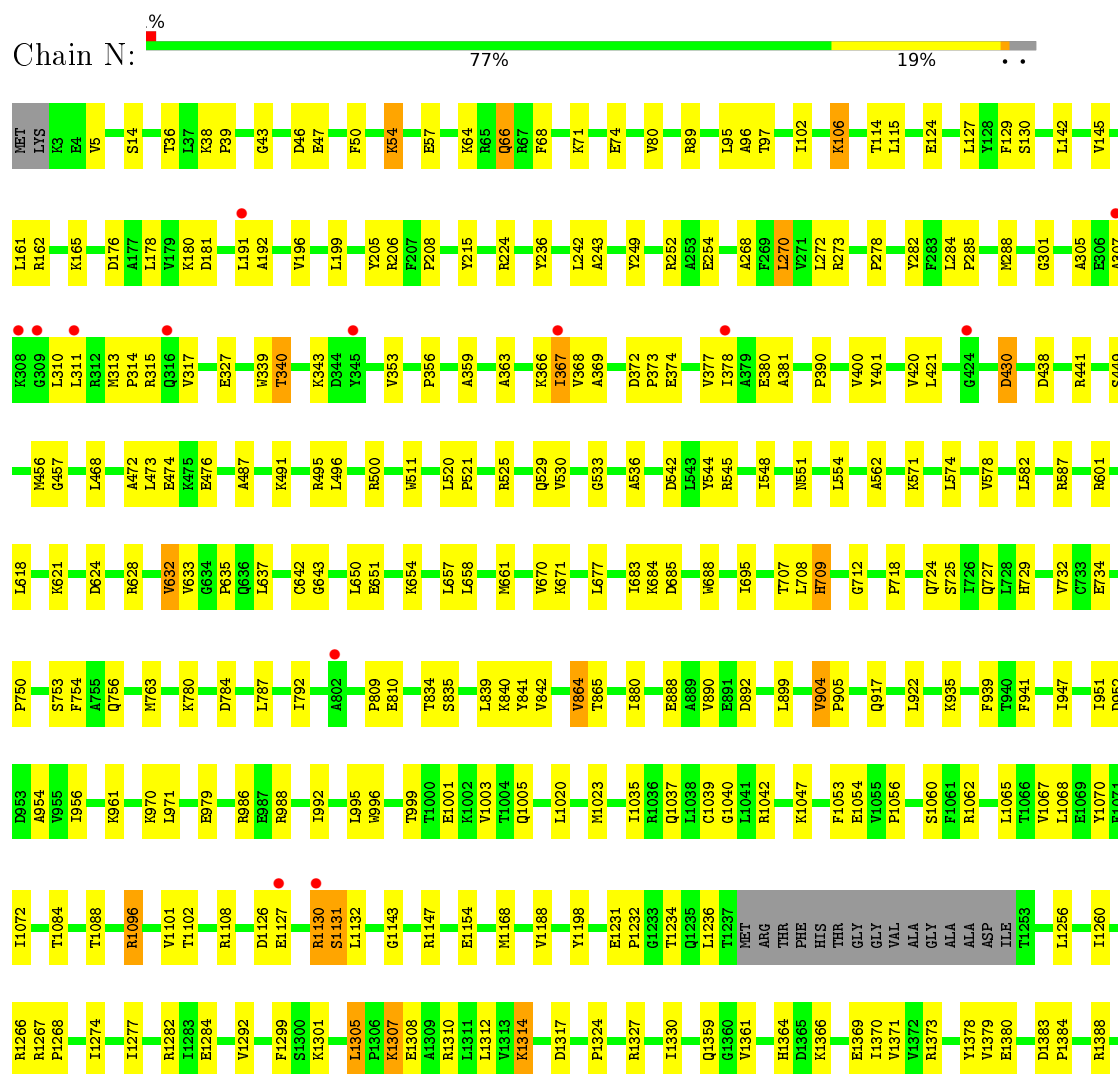


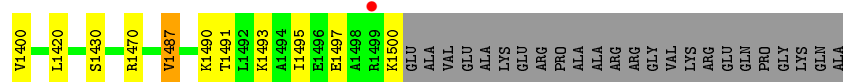
### • Molecule 3: DNA-directed RNA polymerase subunit beta'



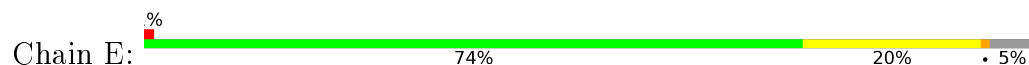


• Molecule 3: DNA-directed RNA polymerase subunit beta'

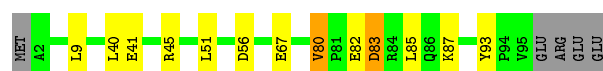
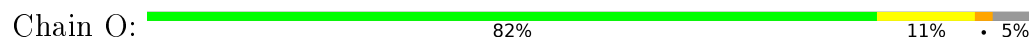




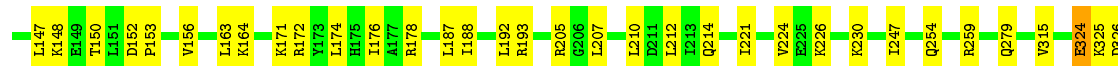
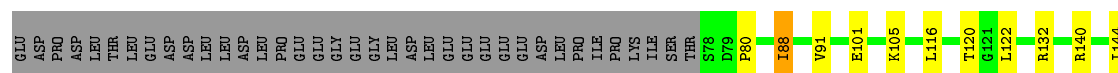
- Molecule 4: DNA-directed RNA polymerase subunit omega



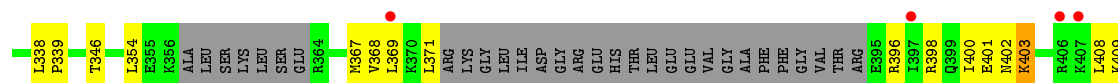
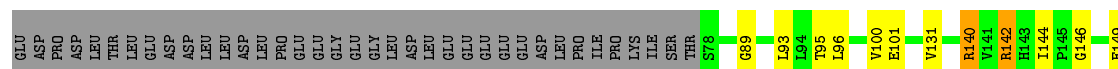
- Molecule 4: DNA-directed RNA polymerase subunit omega



- Molecule 5: RNA polymerase sigma factor SigA

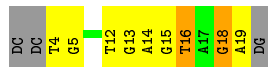
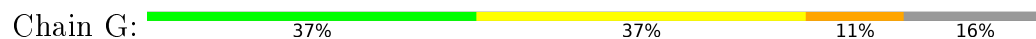


- Molecule 5: RNA polymerase sigma factor SigA





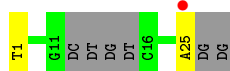
- Molecule 6: DNA (5'-D(\*CP\*C\*TP\*GP\*CP\*AP\*TP\*CP\*CP\*GP\*TP\*GP\*AP\*GP\*TP\*AP\*GP\*AP\*G)-3')



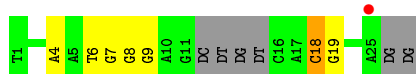
- Molecule 6: DNA (5'-D(\*CP\*C\*TP\*GP\*CP\*AP\*TP\*CP\*CP\*GP\*TP\*GP\*AP\*GP\*TP\*AP\*GP\*AP\*G)-3')



- Molecule 7: DNA (27-MER)



- Molecule 7: DNA (27-MER)





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	185.00Å 103.51Å 296.30Å 90.00° 98.27° 90.00°	Depositor
Resolution (Å)	42.17 – 3.00 49.42 – 2.99	Depositor EDS
% Data completeness (in resolution range)	97.5 (42.17-3.00) 97.7 (49.42-2.99)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.78 (at 3.01Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.201 , 0.254 0.201 , 0.253	Depositor DCC
$R_{free}$ test set	10877 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	48.8	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 31.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	57349	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.42 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.0439e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CTP, ZN, NAD

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	0.29	0/1829	0.53	0/2487
1	B	0.28	0/1781	0.50	0/2420
1	K	0.27	0/1824	0.49	0/2480
1	L	0.28	0/1781	0.50	0/2420
2	C	0.32	0/8913	0.51	0/12053
2	M	0.29	0/8775	0.49	0/11867
3	D	0.31	0/11936	0.50	1/16138 (0.0%)
3	N	0.30	0/11922	0.49	0/16119
4	E	0.31	0/772	0.50	0/1040
4	O	0.28	0/772	0.47	0/1040
5	F	0.29	0/2852	0.46	0/3837
5	P	0.28	0/2614	0.46	0/3516
6	G	0.66	1/368 (0.3%)	1.15	2/567 (0.4%)
6	R	0.53	0/368	1.08	2/567 (0.4%)
7	H	0.57	0/489	1.14	1/752 (0.1%)
7	S	0.55	0/488	1.15	2/750 (0.3%)
All	All	0.31	1/57484 (0.0%)	0.53	8/78053 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	18	DG	O3'-P	-7.08	1.52	1.61

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	16	DT	O4'-C4'-C3'	-7.75	101.35	106.00
7	S	18	DC	O4'-C1'-N1	6.36	112.45	108.00
6	R	16	DT	O4'-C4'-C3'	-5.75	102.20	104.50
6	G	14	DA	O4'-C4'-C3'	-5.62	102.25	104.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	R	14	DA	O4'-C4'-C3'	-5.49	102.30	104.50
7	S	18	DC	O4'-C4'-C3'	-5.42	102.33	104.50
7	H	1	DT	O4'-C1'-N1	5.21	111.64	108.00
3	D	1208	ASP	N-CA-C	-5.11	97.20	111.00

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1797	0	1849	33	0
1	B	1750	0	1802	29	0
1	K	1792	0	1844	39	0
1	L	1750	0	1802	41	0
2	C	8747	0	8858	121	0
2	M	8611	0	8710	169	0
3	D	11730	0	11960	158	0
3	N	11716	0	11949	174	1
4	E	758	0	770	14	0
4	O	758	0	770	7	0
5	F	2807	0	2882	41	0
5	P	2574	0	2643	45	1
6	G	328	0	182	7	0
6	R	328	0	182	3	0
7	H	435	0	238	2	0
7	S	434	0	235	10	0
8	B	1	0	0	0	0
8	D	3	0	0	0	0
8	F	1	0	0	0	0
8	L	1	0	0	0	0
8	N	3	0	0	0	0
8	P	1	0	0	0	0
9	D	2	0	0	0	0
9	N	2	0	0	0	0
10	D	20	0	11	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	N	20	0	11	2	0
11	D	9	0	0	0	0
11	M	9	0	0	0	0
12	D	44	0	24	1	0
13	R	23	0	11	0	0
14	A	23	0	0	0	0
14	B	16	0	0	0	0
14	C	196	0	0	2	0
14	D	244	0	0	7	0
14	E	16	0	0	0	0
14	F	45	0	0	1	0
14	G	8	0	0	0	0
14	H	4	0	0	0	0
14	K	14	0	0	0	0
14	L	13	0	0	1	0
14	M	97	0	0	4	0
14	N	187	0	0	2	0
14	O	12	0	0	0	0
14	P	14	0	0	1	0
14	R	3	0	0	0	0
14	S	3	0	0	0	0
All	All	57349	0	56733	807	1

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 7.

All (807) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:428:ARG:NH2	2:M:447:ALA:O	2.07	0.88
3:N:562:ALA:O	5:P:140:ARG:NH1	2.10	0.84
3:D:124:GLU:OE2	3:D:587:ARG:NH2	2.11	0.84
2:M:674:VAL:HG12	2:M:869:VAL:HB	1.63	0.81
2:C:787:ASP:OD2	2:C:791:ARG:NH2	2.15	0.78
3:N:97:THR:HG21	3:N:571:LYS:HG2	1.67	0.76
2:M:758:ARG:HH21	2:M:788:THR:HB	1.50	0.75
3:N:1495:ILE:HD13	4:O:80:VAL:HG21	1.68	0.75
2:C:807:ARG:NH1	2:C:810:ASP:OD2	2.20	0.75
2:C:165:LEU:HB2	2:C:168:ARG:HG3	1.69	0.74
2:M:802:ARG:HB2	2:M:826:TYR:HB2	1.67	0.74
3:D:1108:ARG:NH2	3:D:1198:TYR:O	2.21	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:711:GLU:HG2	2:M:822:VAL:HG22	1.71	0.72
1:K:179:PHE:HB3	1:K:197:LEU:HD23	1.72	0.71
1:K:180:GLN:NE2	2:M:935:GLY:O	2.24	0.71
2:M:807:ARG:NH1	2:M:810:ASP:OD2	2.24	0.71
2:C:628:PHE:H	2:C:638:ASP:HB3	1.55	0.70
3:N:363:ALA:HB2	3:N:381:ALA:HA	1.74	0.70
3:D:1495:ILE:HG12	4:E:88:GLU:HG3	1.73	0.70
5:P:400:ILE:HA	5:P:403:LYS:HB3	1.73	0.69
2:M:408:ARG:NH1	2:M:456:ALA:O	2.25	0.69
3:N:106:LYS:HE3	3:N:587:ARG:HG3	1.74	0.69
3:N:1310:ARG:HD2	3:N:1327:ARG:HD2	1.73	0.69
3:N:734:GLU:OE2	3:N:780:LYS:NZ	2.25	0.69
2:M:846:LYS:NZ	10:N:2005:C:OP1	2.22	0.69
3:N:270:LEU:HD12	3:N:284:LEU:HD11	1.75	0.68
5:P:265:VAL:O	5:P:269:ASN:ND2	2.25	0.68
2:C:428:ARG:NH2	2:C:447:ALA:O	2.26	0.68
5:F:188:ILE:HD13	5:F:221:ILE:HG12	1.74	0.68
3:D:260:GLU:OE1	3:D:273:ARG:NH1	2.27	0.68
3:N:142:LEU:HB2	3:N:161:LEU:HD11	1.75	0.68
3:D:1495:ILE:HD13	4:E:80:VAL:HG21	1.76	0.68
2:M:628:PHE:H	2:M:638:ASP:HB3	1.58	0.68
1:K:4:SER:O	1:K:189:ARG:NH1	2.25	0.68
2:C:420:ARG:HH22	5:F:324:GLU:HG2	1.59	0.68
2:M:194:VAL:HG22	2:M:221:LEU:HD23	1.76	0.67
3:D:270:LEU:HD12	3:D:284:LEU:HD11	1.75	0.67
3:D:562:ALA:O	5:F:140:ARG:NH1	2.25	0.67
3:D:710:ARG:NH2	14:D:2103:HOH:O	2.26	0.67
2:M:12:VAL:HG13	2:M:13:ILE:HG23	1.76	0.66
5:F:91:VAL:O	5:F:193:ARG:NH2	2.27	0.66
2:M:1034:GLU:OE2	3:N:1096:ARG:NH2	2.29	0.66
2:C:97:ARG:NH1	2:C:110:GLU:OE1	2.28	0.66
2:C:605:LYS:HB2	2:C:612:VAL:HB	1.77	0.66
1:B:108:GLU:HG2	1:B:131:THR:HG22	1.76	0.66
3:D:238:PRO:HD3	3:D:318:ARG:HG3	1.78	0.66
1:L:176:ARG:NH2	3:N:888:GLU:OE1	2.29	0.66
2:M:1095:LEU:HD23	3:N:582:LEU:HD22	1.78	0.66
3:N:367:ILE:HG13	3:N:368:VAL:HG23	1.76	0.65
3:D:1040:GLY:O	3:D:1060:SER:HB3	1.97	0.65
1:K:24:VAL:HG22	1:K:196:THR:HG23	1.77	0.65
1:L:108:GLU:HG2	1:L:131:THR:HG22	1.79	0.65
2:M:30:LEU:HD21	2:M:118:ILE:HG21	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:343:GLN:HG3	2:C:385:PHE:HB2	1.79	0.64
2:M:376:ARG:NH1	2:M:379:GLU:OE1	2.30	0.64
3:D:895:VAL:HG11	3:D:922:LEU:HD21	1.78	0.64
3:N:1147:ARG:NH2	3:N:1369:GLU:OE1	2.30	0.64
3:N:272:LEU:HD22	3:N:282:TYR:HE2	1.63	0.64
2:M:971:LYS:HB3	2:M:986:PRO:HB2	1.80	0.63
3:N:1307:LYS:HD2	3:N:1308:GLU:H	1.63	0.63
3:D:968:ASP:OD1	3:D:1058:ARG:NH2	2.31	0.63
1:K:58:ILE:HG12	1:K:140:MET:HG2	1.79	0.63
3:D:266:GLU:HG3	3:D:314:PRO:HB3	1.81	0.63
5:F:212:LEU:HD22	5:F:247:ILE:HG23	1.79	0.63
5:F:365:GLU:HB2	5:F:404:ALA:HB2	1.79	0.63
2:C:118:ILE:HD11	2:C:344:PHE:HE2	1.64	0.62
1:B:176:ARG:NH2	3:D:888:GLU:OE1	2.32	0.62
4:E:39:VAL:O	4:E:72:ARG:NH1	2.26	0.62
2:M:1110:ASP:OD2	2:M:1114:GLY:N	2.29	0.62
4:O:45:ARG:NH1	4:O:56:ASP:OD2	2.31	0.62
3:D:956:ILE:HD11	3:D:1062:ARG:HG2	1.82	0.62
3:N:474:GLU:HG3	3:N:496:LEU:HD11	1.80	0.62
1:L:83:LYS:NZ	3:N:842:VAL:O	2.33	0.62
1:B:111:ALA:HB3	1:B:125:PRO:HA	1.81	0.62
3:D:970:LYS:HD2	3:D:995:LEU:HD13	1.82	0.61
2:M:437:ARG:NH2	2:M:491:GLU:OE2	2.28	0.61
2:M:11:GLU:HG2	2:M:535:SER:HB2	1.83	0.61
5:P:369:LEU:HD13	5:P:408:LEU:HD22	1.80	0.61
1:A:106:PRO:HG3	1:A:134:GLU:HG2	1.83	0.61
3:N:368:VAL:HB	3:N:377:VAL:HB	1.81	0.61
2:C:797:GLY:O	2:C:829:GLN:NE2	2.34	0.61
2:C:168:ARG:HD3	2:C:268:ASP:HB3	1.82	0.61
2:C:768:THR:OG1	2:C:771:GLU:OE1	2.18	0.61
1:A:180:GLN:NE2	2:C:935:GLY:O	2.34	0.61
2:M:627:ARG:HA	2:M:638:ASP:HB2	1.82	0.61
3:N:970:LYS:HD3	3:N:995:LEU:HD13	1.82	0.61
2:C:1030:GLN:OE1	3:D:628:ARG:NH1	2.34	0.60
2:M:541:SER:O	2:M:545:ASN:ND2	2.30	0.60
3:N:1040:GLY:O	3:N:1060:SER:HB3	2.00	0.60
3:N:273:ARG:HB3	3:N:278:PRO:HA	1.83	0.60
3:D:343:LYS:NZ	3:D:380:GLU:OE1	2.29	0.60
2:C:727:PRO:HB3	2:C:783:ARG:HD3	1.83	0.60
3:N:5:VAL:O	3:N:1470:ARG:NH2	2.34	0.60
4:O:80:VAL:HG13	4:O:85:LEU:HD12	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:ARG:HD3	2:C:934:PHE:CZ	2.36	0.60
3:D:236:TYR:HB2	3:D:319:ALA:HB3	1.84	0.60
3:D:433:GLY:HA2	3:D:449:SER:H	1.67	0.60
4:E:3:GLU:HB3	4:E:65:MET:HE1	1.82	0.60
2:C:816:LYS:HG3	2:C:819:VAL:HG21	1.82	0.60
3:D:566:ILE:HD11	5:F:192:LEU:HD21	1.83	0.60
2:M:1092:LEU:HD13	2:M:1099:VAL:HG21	1.84	0.60
2:M:715:THR:OG1	2:M:718:GLY:O	2.20	0.59
3:N:1108:ARG:NH2	3:N:1198:TYR:O	2.31	0.59
2:C:41:ASN:O	2:C:46:ALA:HB2	2.02	0.59
2:M:872:ASN:ND2	3:N:784:ASP:OD2	2.35	0.59
3:N:643:GLY:HA3	3:N:727:GLN:HB2	1.84	0.59
3:D:1324:PRO:HG3	3:D:1330:ILE:HD11	1.85	0.59
1:L:111:ALA:HB3	1:L:125:PRO:HA	1.84	0.59
3:D:418:GLY:HA2	3:D:428:LYS:HD3	1.83	0.59
1:L:77:GLU:O	1:L:81:ASN:ND2	2.36	0.59
2:M:74:GLY:HA3	2:M:93:PRO:HG2	1.85	0.59
3:N:954:ALA:O	3:N:1062:ARG:NH2	2.35	0.59
3:N:1364:HIS:ND1	3:N:1366:LYS:HG2	2.18	0.59
2:M:808:ARG:NH2	5:P:305:GLU:OE2	2.36	0.59
2:M:628:PHE:H	2:M:638:ASP:CB	2.16	0.58
2:M:35:PRO:HG2	2:M:38:LYS:HB2	1.85	0.58
2:M:936:VAL:HG11	2:M:959:PRO:HB2	1.84	0.58
1:K:48:ILE:HD12	1:K:213:GLN:HG3	1.85	0.58
2:C:397:GLU:HG3	2:C:631:SER:HB2	1.85	0.58
3:N:208:PRO:HA	3:N:390:PRO:HA	1.84	0.58
2:C:937:ASP:OD1	2:C:939:ARG:HD3	2.03	0.58
3:D:1096:ARG:NH1	3:D:1440:PHE:O	2.36	0.58
2:M:680:ASP:OD2	2:M:978:ARG:NH2	2.36	0.58
3:N:57:GLU:HG3	3:N:64:LYS:HB3	1.86	0.58
3:D:904:VAL:HG22	3:D:905:PRO:HD2	1.86	0.58
3:D:486:ARG:HA	3:D:489:ARG:HH21	1.69	0.58
3:N:206:ARG:NH2	5:P:101:GLU:OE2	2.37	0.58
2:C:176:VAL:HG22	2:C:182:VAL:HG12	1.85	0.57
2:M:370:ALA:O	5:P:280:GLN:NE2	2.37	0.57
3:D:1383:ASP:HB3	3:D:1416:ALA:HB3	1.86	0.57
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.87	0.57
1:K:103:ALA:HB1	1:K:107:LYS:HD3	1.86	0.57
2:M:637:LEU:HG	2:M:659:PRO:HG3	1.87	0.57
1:A:112:ARG:HG3	1:A:125:PRO:HB2	1.87	0.57
1:A:209:GLU:O	1:A:213:GLN:HG2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:658:LEU:HA	3:N:661:MET:HE3	1.86	0.57
1:L:112:ARG:HG3	1:L:125:PRO:HB2	1.86	0.56
2:M:283:ILE:HD13	2:M:305:PRO:HG3	1.87	0.56
2:M:768:THR:OG1	2:M:771:GLU:OE1	2.24	0.56
2:M:22:GLN:NE2	14:M:1303:HOH:O	2.37	0.56
2:M:405:ARG:HD3	2:M:566:THR:HG21	1.86	0.56
2:C:628:PHE:H	2:C:638:ASP:CB	2.18	0.56
2:C:674:VAL:HG12	2:C:869:VAL:HB	1.88	0.56
3:D:840:LYS:O	14:D:2101:HOH:O	2.18	0.56
3:D:1068:LEU:O	3:D:1072:ILE:HG12	2.05	0.56
7:H:25:DA:OP2	7:H:25:DA:H8	1.88	0.56
2:M:189:ARG:HH22	2:M:244:PRO:HD3	1.71	0.56
3:N:356:PRO:HG2	3:N:359:ALA:HB2	1.86	0.56
2:C:182:VAL:HG23	2:C:193:LEU:HB3	1.88	0.56
3:N:89:ARG:NH1	14:N:2103:HOH:O	2.33	0.56
3:N:787:LEU:HD21	3:N:947:ILE:HG21	1.88	0.56
3:D:1100:ASP:OD2	3:D:1463:LYS:NZ	2.34	0.56
2:M:714:ASP:OD2	2:M:808:ARG:NH1	2.39	0.56
5:F:163:LEU:HD13	5:F:174:LEU:HD13	1.86	0.56
3:D:236:TYR:CD2	3:D:322:VAL:HG21	2.41	0.55
2:M:18:LEU:HB2	2:M:404:LEU:HD11	1.88	0.55
2:M:324:ASP:HB3	2:M:327:HIS:HB2	1.88	0.55
2:C:513:VAL:HG13	2:C:524:VAL:HG23	1.88	0.55
3:D:106:LYS:HE3	3:D:587:ARG:HG3	1.87	0.55
2:M:939:ARG:HG2	2:M:982:PRO:HD3	1.88	0.55
1:B:216:GLU:OE1	1:B:219:ARG:NH2	2.36	0.55
2:M:777:ILE:HG23	5:P:412:GLU:HG2	1.88	0.55
3:D:1105:ILE:HG23	3:D:1199:GLY:HA2	1.89	0.55
5:F:361:LEU:HB3	5:F:365:GLU:HG3	1.89	0.55
5:F:393:THR:HG22	5:F:395:GLU:H	1.70	0.55
5:P:265:VAL:HG12	5:P:269:ASN:HD21	1.71	0.55
2:M:513:VAL:HG13	2:M:524:VAL:HG23	1.88	0.55
5:P:368:VAL:HA	5:P:371:LEU:HD12	1.89	0.55
2:C:708:TYR:HB3	2:C:790:LEU:HD21	1.89	0.55
3:D:890:VAL:HB	3:D:922:LEU:HD13	1.88	0.55
5:F:188:ILE:HG12	5:F:224:VAL:HG21	1.89	0.55
10:N:2005:C:O2	6:R:15:DG:N2	2.35	0.55
1:A:70:GLY:N	2:C:607:ASP:OD1	2.37	0.55
2:C:405:ARG:HD3	2:C:566:THR:HG21	1.88	0.55
2:M:243:ARG:NH1	7:S:9:DG:O6	2.40	0.55
1:A:20:TYR:OH	1:A:198:ARG:HD2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:670:GLN:HG2	2:C:699:PHE:CD2	2.41	0.55
1:K:198:ARG:HD3	2:M:934:PHE:CZ	2.40	0.55
2:M:937:ASP:OD1	2:M:939:ARG:HD3	2.07	0.55
2:M:169:GLY:HA3	2:M:267:TYR:HD1	1.71	0.54
3:N:1324:PRO:HG3	3:N:1330:ILE:HD11	1.88	0.54
1:A:179:PHE:HB3	1:A:197:LEU:HD23	1.88	0.54
2:C:930:LYS:HE3	2:C:935:GLY:HA2	1.90	0.54
1:K:112:ARG:HG3	1:K:125:PRO:HB2	1.88	0.54
3:D:1364:HIS:ND1	3:D:1366:LYS:HG2	2.20	0.54
3:N:1126:ASP:OD2	3:N:1127:GLU:N	2.40	0.54
3:D:241:ILE:HA	3:D:312:ARG:HB3	1.88	0.54
2:M:405:ARG:HD2	2:M:442:GLU:OE2	2.08	0.54
3:N:236:TYR:HB3	3:N:313:MET:HG3	1.90	0.54
3:N:996:TRP:CD2	3:N:1056:PRO:HG3	2.43	0.54
3:N:1236:LEU:HA	3:N:1359:GLN:HG3	1.90	0.54
3:N:904:VAL:HG22	3:N:905:PRO:HD2	1.90	0.54
3:D:114:THR:HG23	3:D:495:ARG:HG2	1.89	0.54
2:M:274:ARG:NH2	2:M:285:LEU:O	2.41	0.54
3:D:356:PRO:HG2	3:D:359:ALA:HB2	1.89	0.54
6:G:4:DT:H2"	6:G:5:DG:C8	2.42	0.54
3:D:171:LEU:HD12	3:D:390:PRO:HG2	1.89	0.53
3:N:1277:ILE:HD11	3:N:1301:LYS:HG3	1.90	0.53
1:L:128:HIS:CE1	1:L:131:THR:HG23	2.44	0.53
1:L:64:GLU:HA	1:L:165:ILE:HD13	1.89	0.53
2:M:146:VAL:HG22	2:M:162:ILE:HG12	1.90	0.53
2:M:880:MET:SD	3:N:1037:GLN:NE2	2.82	0.53
3:D:371:ILE:HG23	5:F:230:LYS:HD2	1.90	0.53
2:M:333:ILE:HD11	2:M:467:ILE:HD11	1.90	0.53
1:B:132:LEU:HD21	1:B:138:LEU:HB2	1.90	0.53
2:C:872:ASN:ND2	3:D:784:ASP:OD1	2.40	0.53
3:D:1426:LYS:O	3:D:1430:SER:OG	2.21	0.53
3:N:999:THR:O	3:N:1003:VAL:HG23	2.09	0.53
3:N:529:GLN:NE2	3:N:533:GLY:O	2.41	0.53
3:N:124:GLU:OE2	3:N:587:ARG:NH2	2.42	0.53
3:N:988:ARG:NH2	3:N:1054:GLU:OE2	2.39	0.53
2:C:462:ASP:HB3	2:C:468:ARG:HD2	1.90	0.53
2:C:627:ARG:HA	2:C:638:ASP:HB2	1.91	0.53
2:M:15:LEU:HD11	2:M:583:LEU:HD11	1.91	0.53
3:N:285:PRO:HG2	3:N:311:LEU:HD22	1.89	0.53
2:C:118:ILE:HD11	2:C:344:PHE:CE2	2.42	0.53
3:D:553:ARG:HD2	3:D:570:GLU:OE2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1056:LYS:HE2	3:D:751:LEU:HG	1.91	0.53
2:C:936:VAL:HG11	2:C:959:PRO:HB2	1.90	0.53
3:N:367:ILE:HG23	3:N:377:VAL:HG12	1.90	0.53
3:D:231:VAL:O	3:D:236:TYR:OH	2.25	0.52
5:P:205:ARG:HG3	5:P:251:ILE:HD13	1.92	0.52
5:F:144:ILE:HB	5:F:147:LEU:HD13	1.90	0.52
1:A:216:GLU:OE2	1:A:219:ARG:NH2	2.43	0.52
2:C:13:ILE:HD13	2:C:483:VAL:HG11	1.92	0.52
2:C:397:GLU:H	2:C:633:GLN:HE22	1.56	0.52
6:G:18:DG:H2'	6:G:19:DA:C8	2.44	0.52
2:C:1050:GLN:O	2:C:1054:THR:OG1	2.21	0.52
2:C:232:GLU:HG3	2:C:250:ARG:HE	1.73	0.52
3:D:208:PRO:HA	3:D:390:PRO:HA	1.91	0.52
2:M:67:ASP:OD1	2:M:68:PHE:N	2.42	0.52
3:N:956:ILE:HD11	3:N:1062:ARG:HG2	1.92	0.52
2:C:200:LEU:HD13	2:C:300:ASP:HB2	1.91	0.52
1:L:83:LYS:HE2	1:L:168:ASP:HB2	1.90	0.52
2:C:607:ASP:HB2	2:C:610:ARG:HH11	1.75	0.52
3:N:39:PRO:HG2	3:N:47:GLU:HG3	1.91	0.52
3:N:487:ALA:O	3:N:491:LYS:HG2	2.10	0.52
3:D:135:LEU:HD22	3:D:455:ARG:HE	1.73	0.52
3:N:658:LEU:HD23	3:N:661:MET:HE1	1.92	0.52
2:M:690:ILE:HG13	2:M:852:ILE:HG23	1.92	0.51
3:N:1068:LEU:O	3:N:1072:ILE:HG12	2.10	0.51
3:N:181:ASP:HB2	3:N:205:TYR:CD1	2.46	0.51
2:M:915:LYS:NZ	3:N:952:ASP:OD2	2.44	0.51
2:C:177:GLU:HG3	2:C:178:PRO:HD2	1.91	0.51
2:C:693:GLU:HG2	2:C:855:VAL:HB	1.92	0.51
3:D:644:LEU:HD12	3:D:645:PRO:HD2	1.92	0.51
2:M:92:ALA:HB2	2:M:120:LEU:HD11	1.92	0.51
2:M:189:ARG:NH2	2:M:241:LEU:O	2.42	0.51
2:M:861:LEU:HD12	2:M:865:THR:HB	1.92	0.51
1:K:36:LEU:HD11	1:L:221:HIS:HB3	1.93	0.51
1:L:57:TYR:CE1	1:L:163:ASN:HB2	2.46	0.51
3:N:268:ALA:HB3	3:N:284:LEU:HD12	1.93	0.51
3:N:520:LEU:HD12	3:N:521:PRO:HD2	1.93	0.51
3:D:314:PRO:HB2	3:D:317:VAL:HG12	1.93	0.51
2:M:169:GLY:HA3	2:M:267:TYR:CD1	2.46	0.51
2:M:773:LEU:HD23	5:P:354:LEU:HD13	1.93	0.51
1:A:218:LEU:HD23	1:B:222:LEU:HD21	1.91	0.51
2:C:324:ASP:HB3	2:C:327:HIS:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:ARG:HG3	1:B:125:PRO:HB2	1.91	0.51
2:C:545:ASN:HB3	2:C:583:LEU:HD22	1.93	0.51
3:D:356:PRO:HB3	3:D:441:ARG:HA	1.93	0.51
2:M:614:ARG:NH2	2:M:618:GLY:O	2.44	0.51
3:N:224:ARG:NH1	3:N:254:GLU:OE2	2.38	0.51
1:L:80:LEU:HD21	3:N:842:VAL:HG12	1.93	0.51
1:A:97:VAL:HG12	1:A:99:LEU:HD12	1.93	0.50
1:K:39:PRO:HG3	1:L:39:PRO:HG3	1.92	0.50
2:M:172:ILE:HG12	2:M:186:VAL:HG22	1.93	0.50
2:M:584:GLU:N	2:M:584:GLU:OE2	2.44	0.50
3:N:14:SER:HB3	3:N:511:TRP:CE2	2.46	0.50
2:C:690:ILE:HG22	2:C:869:VAL:HG22	1.93	0.50
3:D:954:ALA:O	3:D:1062:ARG:NH2	2.44	0.50
5:P:409:LYS:HA	5:P:412:GLU:HG3	1.93	0.50
3:D:1042:ARG:HD2	3:D:1061:PHE:CZ	2.46	0.50
1:L:56:VAL:HG22	1:L:142:VAL:HG12	1.93	0.50
2:M:1009:SER:HB3	3:N:651:GLU:O	2.11	0.50
3:N:50:PHE:O	3:N:89:ARG:HD2	2.10	0.50
3:D:1143:GLY:O	3:D:1147:ARG:HD2	2.11	0.50
3:D:945:SER:OG	3:D:947:ILE:HG12	2.11	0.50
1:K:220:GLU:O	1:K:223:THR:HB	2.12	0.50
2:M:286:SER:OG	2:M:287:GLY:N	2.43	0.50
2:M:535:SER:O	2:M:538:GLN:HG2	2.12	0.50
3:D:1495:ILE:HG22	3:D:1499:ARG:HD2	1.94	0.50
3:D:128:TYR:OH	3:D:579:ASP:OD2	2.22	0.50
3:N:545:ARG:NH1	5:P:254:GLN:O	2.43	0.50
2:C:436:GLY:HA2	2:C:538:GLN:O	2.12	0.50
2:C:134:ARG:NH1	2:C:392:SER:O	2.43	0.49
1:K:209:GLU:O	1:K:213:GLN:HG2	2.12	0.49
3:D:1444:THR:O	3:D:1448:THR:HG23	2.11	0.49
1:K:219:ARG:HG3	14:L:2111:HOH:O	2.11	0.49
1:A:150:TYR:CD1	2:C:696:LYS:HG2	2.47	0.49
1:A:39:PRO:HG3	1:B:39:PRO:HG3	1.94	0.49
3:D:658:LEU:HA	3:D:661:MET:HE3	1.95	0.49
12:D:2008:NAD:H62A	6:G:16:DT:H3	1.59	0.49
2:M:617:ASP:HB2	2:M:619:ARG:HG2	1.92	0.49
3:N:890:VAL:HB	3:N:922:LEU:HD13	1.93	0.49
3:D:657:LEU:HG	3:D:661:MET:HE2	1.93	0.49
2:M:603:VAL:HG11	2:M:606:VAL:HG23	1.95	0.49
2:M:536:PRO:HB3	3:N:1067:VAL:HG21	1.94	0.49
3:N:1130:ARG:O	3:N:1131:SER:HB3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:131:VAL:HG13	5:P:178:ARG:HD3	1.94	0.49
5:P:152:ASP:N	5:P:152:ASP:OD1	2.45	0.49
2:C:229:MET:HB2	2:C:233:GLU:HB2	1.95	0.49
3:D:1491:THR:O	3:D:1495:ILE:HG13	2.13	0.49
3:N:750:PRO:HG2	3:N:756:GLN:NE2	2.27	0.49
3:D:489:ARG:NH1	3:D:1391:GLU:OE1	2.46	0.49
3:D:801:GLY:O	3:D:804:LEU:HG	2.13	0.49
3:N:366:LYS:HD3	3:N:369:ALA:HB2	1.94	0.49
5:P:193:ARG:HB3	7:S:7:DG:H5"	1.95	0.49
2:C:1042:ALA:HB3	3:D:710:ARG:HB3	1.95	0.49
3:N:208:PRO:HG2	3:N:353:VAL:HG21	1.95	0.49
1:A:57:TYR:CD1	1:A:161:ARG:HD2	2.48	0.48
2:C:711:GLU:HG2	2:C:822:VAL:HG22	1.94	0.48
3:D:218:LYS:HG2	3:D:338:GLU:HG2	1.95	0.48
3:D:959:GLU:HB3	3:D:963:TYR:CE1	2.47	0.48
1:K:56:VAL:HG21	1:K:82:LEU:HD13	1.94	0.48
2:M:397:GLU:HG3	2:M:631:SER:HB2	1.94	0.48
2:M:673:LEU:HD23	2:M:867:VAL:HA	1.95	0.48
2:M:462:ASP:HB3	2:M:468:ARG:HD2	1.94	0.48
2:M:47:ALA:O	2:M:51:THR:HG23	2.12	0.48
2:C:1067:TYR:OH	3:D:674:ARG:NH1	2.47	0.48
1:K:99:LEU:HD21	1:K:122:ILE:HD11	1.94	0.48
3:N:102:ILE:HD11	3:N:587:ARG:HB2	1.95	0.48
3:N:317:VAL:HB	3:N:339:TRP:HB3	1.95	0.48
2:C:324:ASP:O	2:C:330:ASN:ND2	2.41	0.48
1:L:57:TYR:HE1	1:L:163:ASN:HB2	1.76	0.48
2:M:668:LEU:N	14:M:1306:HOH:O	2.42	0.48
3:N:215:TYR:HE1	3:N:381:ALA:H	1.60	0.48
3:N:657:LEU:HG	3:N:661:MET:HE2	1.95	0.48
1:L:94:LEU:HD21	1:L:97:VAL:HG22	1.95	0.48
1:A:70:GLY:HA3	1:A:136:GLY:HA2	1.95	0.48
1:B:100:LEU:HG	1:B:141:GLU:HG2	1.96	0.48
1:K:225:PHE:HE1	1:L:36:LEU:HD13	1.78	0.48
2:C:976:ASP:OD2	2:C:978:ARG:NH1	2.47	0.48
3:D:1237:THR:H	3:D:1359:GLN:NE2	2.12	0.48
3:N:1088:THR:HA	3:N:1234:THR:HG22	1.95	0.48
5:P:316:SER:O	5:P:319:THR:OG1	2.27	0.48
5:F:187:LEU:HD23	5:F:224:VAL:HG13	1.96	0.48
1:L:143:ARG:NE	1:L:145:ASP:OD1	2.47	0.48
3:N:68:PHE:HB2	3:N:80:VAL:HG11	1.96	0.48
3:N:695:ILE:HD12	3:N:718:PRO:HG2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:218:LEU:HG	1:L:222:LEU:HD11	1.95	0.48
2:M:1009:SER:O	3:N:624:ASP:HB3	2.14	0.48
2:M:497:ALA:HB3	2:M:532:MET:HG3	1.94	0.48
2:C:1102:LEU:HB2	3:D:7:LYS:HB2	1.95	0.48
3:D:208:PRO:HG2	3:D:353:VAL:HG21	1.95	0.48
3:D:227:LEU:HD13	3:D:331:VAL:HB	1.95	0.48
3:N:500:ARG:NH1	3:N:1388:ARG:O	2.43	0.48
2:M:238:LEU:HA	2:M:241:LEU:HD12	1.95	0.47
2:M:740:GLU:HB3	2:M:805:ARG:NH1	2.29	0.47
2:C:133:ASP:HB3	2:C:395:LYS:HD3	1.95	0.47
1:B:83:LYS:HE2	1:B:168:ASP:HB2	1.95	0.47
2:C:1006:HIS:HB2	2:C:1024:LYS:HG3	1.96	0.47
3:D:236:TYR:HD2	3:D:322:VAL:HG21	1.79	0.47
14:D:2102:HOH:O	4:E:37:ASN:HB2	2.15	0.47
1:B:128:HIS:CE1	1:B:131:THR:HG23	2.49	0.47
2:C:35:PRO:HG2	2:C:38:LYS:HD2	1.95	0.47
2:C:74:GLY:HA3	2:C:93:PRO:HG2	1.96	0.47
3:N:542:ASP:OD2	3:N:545:ARG:NH2	2.47	0.47
1:L:153:ALA:HA	1:L:156:HIS:NE2	2.29	0.47
1:L:150:TYR:CE1	1:L:170:VAL:HG22	2.50	0.47
2:M:195:LEU:HA	2:M:226:VAL:HG11	1.96	0.47
2:M:246:ASP:OD2	2:M:252:LYS:NZ	2.43	0.47
2:M:595:LEU:HD21	2:M:623:TYR:HB3	1.96	0.47
2:M:290:LEU:HD23	2:M:302:VAL:HG21	1.96	0.47
3:N:129:PHE:CD1	3:N:456:MET:HB3	2.49	0.47
3:N:165:LYS:HE2	3:N:199:LEU:HD22	1.96	0.47
2:C:224:GLU:HG2	2:C:225:SER:H	1.80	0.47
3:D:569:ASN:ND2	5:F:214:GLN:OE1	2.32	0.47
1:L:71:VAL:HG22	1:L:132:LEU:HG	1.96	0.47
5:P:89:GLY:HA3	7:S:7:DG:C6	2.49	0.47
2:M:216:GLU:HA	2:M:219:GLN:HE21	1.78	0.47
2:M:337:GLY:O	2:M:341:THR:HG23	2.15	0.47
1:B:213:GLN:O	1:B:217:ILE:HG13	2.14	0.47
3:N:71:LYS:NZ	3:N:74:GLU:OE2	2.47	0.47
3:N:890:VAL:HG23	3:N:892:ASP:H	1.80	0.47
1:L:113:ASP:OD2	1:L:113:ASP:N	2.48	0.47
2:M:24:GLU:HG3	2:M:27:ARG:HH21	1.79	0.47
1:A:25:LEU:HD23	1:A:28:LEU:HD21	1.96	0.47
3:D:101:HIS:HB3	3:D:104:PHE:HD2	1.80	0.47
6:G:15:DG:H2'	6:G:16:DT:C6	2.50	0.47
2:M:1065:ALA:HB1	2:M:1077:PRO:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:40:GLU:OE1	2:M:41:ASN:N	2.48	0.47
2:C:28:ARG:NH2	2:C:42:VAL:HG11	2.30	0.46
3:N:1380:GLU:HB2	3:N:1420:LEU:HD22	1.96	0.46
1:A:133:GLU:HG2	1:A:134:GLU:N	2.31	0.46
2:C:63:GLY:HA3	2:C:100:LEU:HD11	1.96	0.46
2:C:595:LEU:HB3	2:C:656:ALA:HB3	1.98	0.46
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.96	0.46
2:M:124:ASP:HB3	2:M:592:LEU:HD12	1.97	0.46
5:P:321:ILE:HA	5:P:321:ILE:HD12	1.76	0.46
1:A:58:ILE:HG12	1:A:140:MET:HG2	1.97	0.46
2:C:597:ALA:HB2	2:C:655:LEU:HD21	1.97	0.46
3:D:629:SER:OG	3:D:630:VAL:N	2.48	0.46
3:D:734:GLU:OE2	3:D:780:LYS:NZ	2.49	0.46
2:M:859:PRO:O	2:M:867:VAL:HG22	2.16	0.46
3:N:1232:PRO:HG3	3:N:1361:VAL:HG11	1.97	0.46
3:N:96:ALA:HB3	3:N:554:LEU:HD23	1.98	0.46
2:C:5:ARG:HB3	2:C:902:ILE:HB	1.97	0.46
3:D:368:VAL:HB	3:D:377:VAL:HB	1.98	0.46
1:A:91:ASN:HA	1:A:92:PRO:HD3	1.83	0.46
2:M:710:ILE:HD12	2:M:790:LEU:HB2	1.96	0.46
2:M:948:GLU:OE2	2:M:955:PRO:HA	2.15	0.46
3:N:1047:LYS:HG2	3:N:1053:PHE:CZ	2.51	0.46
3:N:1147:ARG:HD3	3:N:1188:VAL:HG11	1.98	0.46
3:N:372:ASP:HA	3:N:373:PRO:HD3	1.85	0.46
3:D:1147:ARG:NH2	3:D:1369:GLU:OE1	2.44	0.46
2:C:280:LYS:HE3	2:C:309:TYR:CZ	2.51	0.46
3:N:215:TYR:CZ	3:N:380:GLU:HB2	2.51	0.46
5:P:188:ILE:HD13	5:P:221:ILE:HG12	1.97	0.46
2:C:717:LEU:HD22	2:C:763:GLY:HA2	1.98	0.46
4:E:57:ASP:O	4:E:63:TRP:NE1	2.46	0.46
2:M:97:ARG:HG3	2:M:112:GLU:HG3	1.98	0.46
2:C:206:THR:HG23	2:C:209:ARG:NH1	2.31	0.46
3:D:103:TRP:O	3:D:107:ASP:HB3	2.15	0.46
1:K:226:SER:O	1:K:228:PRO:HD3	2.16	0.46
5:F:116:LEU:HD11	5:F:174:LEU:HA	1.99	0.46
1:K:32:PHE:HA	1:K:35:THR:HB	1.97	0.46
3:N:996:TRP:CE2	3:N:1056:PRO:HG3	2.51	0.46
1:B:110:LYS:HD3	1:B:128:HIS:HA	1.98	0.45
3:D:1084:THR:O	3:D:1088:THR:HG23	2.16	0.45
3:D:271:VAL:HG22	3:D:281:THR:HG23	1.96	0.45
3:D:81:THR:OG1	3:D:82:LYS:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:195:LEU:O	2:M:199:VAL:HG23	2.17	0.45
2:M:657:ASP:OD2	2:M:663:ASN:N	2.48	0.45
2:M:874:LEU:HD23	3:N:1023:MET:SD	2.56	0.45
3:N:1101:VAL:HG13	3:N:1102:THR:HG23	1.97	0.45
3:N:288:MET:HE2	3:N:305:ALA:HB3	1.98	0.45
3:N:685:ASP:HA	3:N:688:TRP:HD1	1.81	0.45
1:K:99:LEU:HB3	1:K:114:PHE:CD2	2.52	0.45
2:C:757:GLY:HA2	2:C:789:SER:OG	2.16	0.45
5:F:370:LYS:HB3	5:F:376:ILE:HG12	1.97	0.45
7:H:25:DA:C8	7:H:25:DA:OP2	2.69	0.45
3:N:536:ALA:HA	5:P:315:VAL:O	2.17	0.45
3:D:409:VAL:HG13	3:D:435:VAL:HG11	1.97	0.45
3:D:1480:PHE:O	4:E:18:ARG:NH2	2.50	0.45
2:M:1083:GLU:OE1	2:M:1086:ARG:NH1	2.48	0.45
2:M:12:VAL:HG11	2:M:472:ARG:HD3	1.98	0.45
3:N:114:THR:HG23	3:N:495:ARG:HG2	1.98	0.45
2:C:1038:TRP:CE2	3:D:1099:VAL:HG11	2.51	0.45
1:L:150:TYR:HE1	1:L:170:VAL:HG22	1.82	0.45
1:L:185:ARG:NH1	1:L:187:GLY:O	2.50	0.45
2:M:343:GLN:HG3	2:M:385:PHE:HB2	1.99	0.45
2:M:11:GLU:OE2	2:M:537:LYS:HE2	2.17	0.45
2:M:944:LEU:HD21	2:M:963:LEU:HD23	1.99	0.45
2:C:64:LEU:HD23	2:C:103:LYS:HD3	1.98	0.45
3:N:809:PRO:HB3	3:N:839:LEU:HD13	1.97	0.45
5:P:142:ARG:HE	5:P:142:ARG:H	1.62	0.45
3:D:963:TYR:CD2	3:D:1002:LYS:HD3	2.52	0.45
3:D:307:ALA:HB1	3:D:311:LEU:HD21	1.98	0.45
4:E:51:LEU:H	4:E:51:LEU:HD12	1.82	0.45
5:F:164:LYS:HA	5:F:171:LYS:HE3	1.97	0.45
1:L:110:LYS:HD2	1:L:126:ASP:O	2.17	0.45
2:M:41:ASN:O	2:M:46:ALA:HB2	2.17	0.45
2:C:976:ASP:OD1	2:C:978:ARG:HD3	2.17	0.45
3:D:273:ARG:HH21	3:D:278:PRO:HD3	1.81	0.45
3:D:346:ARG:HG2	3:D:348:GLN:NE2	2.32	0.45
3:D:593:ASN:HB2	14:D:2134:HOH:O	2.17	0.45
5:F:207:LEU:HD21	5:F:254:GLN:HB2	1.98	0.45
2:M:236:ILE:O	2:M:240:THR:HG23	2.17	0.45
3:N:178:LEU:HG	3:N:192:ALA:HA	1.99	0.45
2:C:862:PRO:HA	2:C:975:TYR:CE2	2.52	0.45
3:D:1236:LEU:HA	3:D:1359:GLN:HG3	1.99	0.45
1:L:41:ARG:HG3	1:L:177:VAL:HB	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:162:ARG:O	3:N:449:SER:HB2	2.17	0.45
3:N:243:ALA:HB3	3:N:311:LEU:HD12	1.99	0.45
3:N:473:LEU:HD21	3:N:495:ARG:HH21	1.82	0.45
3:N:729:HIS:O	3:N:732:VAL:HG22	2.17	0.45
2:C:36:PRO:HB3	2:C:70:GLU:HB2	1.98	0.45
1:K:105:GLY:O	1:K:107:LYS:N	2.49	0.45
3:N:1143:GLY:O	3:N:1147:ARG:HD2	2.15	0.45
3:N:215:TYR:O	3:N:340:THR:HA	2.16	0.45
3:N:840:LYS:HE3	3:N:841:TYR:CZ	2.52	0.45
2:M:778:PHE:CD1	5:P:422:LEU:HD22	2.52	0.45
1:B:57:TYR:CG	1:B:161:ARG:HD2	2.52	0.44
2:C:351:LEU:HD12	2:C:375:SER:HA	1.98	0.44
3:D:536:ALA:HA	5:F:315:VAL:O	2.18	0.44
3:N:1020:LEU:HB3	3:N:1035:ILE:HD12	1.99	0.44
3:N:1102:THR:HG21	3:N:1371:VAL:HG22	1.99	0.44
3:N:401:TYR:OH	3:N:430:ASP:OD2	2.33	0.44
5:P:142:ARG:HE	5:P:142:ARG:N	2.15	0.44
5:P:212:LEU:HD22	5:P:247:ILE:HG23	1.99	0.44
2:C:146:VAL:HG22	2:C:162:ILE:HG12	2.00	0.44
3:D:235:ALA:HA	3:D:322:VAL:HG23	1.99	0.44
3:D:637:LEU:HD13	3:D:642:CYS:HA	1.99	0.44
2:M:561:GLY:O	2:M:565:GLN:HG3	2.17	0.44
2:C:1037:VAL:HG13	2:C:1049:LEU:HD11	1.98	0.44
1:L:220:GLU:O	1:L:223:THR:OG1	2.24	0.44
2:M:76:PRO:HA	2:M:77:PRO:HD2	1.89	0.44
3:N:1314:LYS:HG3	3:N:1317:ASP:OD2	2.18	0.44
3:N:307:ALA:HB1	3:N:311:LEU:HD21	1.99	0.44
5:P:144:ILE:HG22	5:P:146:GLY:H	1.82	0.44
5:P:319:THR:HA	5:P:320:PRO:HD3	1.85	0.44
2:M:243:ARG:HH12	7:S:9:DG:H1	1.64	0.44
3:D:842:VAL:HG22	3:D:865:THR:HB	1.98	0.44
5:F:88:ILE:HD12	5:F:88:ILE:HA	1.69	0.44
2:M:736:ASP:O	2:M:744:ARG:HG2	2.18	0.44
2:M:896:PHE:HB2	2:M:921:ALA:HB1	1.99	0.44
3:N:38:LYS:HA	3:N:38:LYS:HD3	1.83	0.44
5:P:93:LEU:HD21	5:P:193:ARG:HD2	1.98	0.44
3:D:483:HIS:CG	3:D:484:PRO:HD2	2.53	0.44
1:A:150:TYR:CE2	1:A:152:PRO:HG3	2.53	0.44
3:D:1366:LYS:O	3:D:1370:ILE:HG13	2.17	0.44
3:D:1379:VAL:HG21	3:D:1400:VAL:HG11	1.99	0.44
2:M:328:LEU:HD12	2:M:433:THR:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1084:THR:O	3:N:1088:THR:HG23	2.17	0.44
3:D:483:HIS:CE1	3:D:488:ARG:HD3	2.53	0.44
6:G:12:DT:H2'	6:G:13:DG:C8	2.53	0.44
3:N:314:PRO:HG2	3:N:317:VAL:HG13	1.99	0.44
5:P:398:ARG:HA	5:P:401:GLU:HB3	1.99	0.44
2:C:1110:ASP:OD2	2:C:1114:GLY:N	2.43	0.44
2:C:172:ILE:HD13	2:C:184:MET:HE3	2.00	0.44
2:C:617:ASP:OD2	2:C:619:ARG:HG2	2.17	0.44
3:D:1493:LYS:HD3	3:D:1493:LYS:HA	1.74	0.44
1:L:57:TYR:CG	1:L:161:ARG:HD2	2.53	0.44
2:M:184:MET:HE1	2:M:196:LEU:HD13	2.00	0.44
2:M:850:ALA:HB1	3:N:632:VAL:HG13	1.98	0.44
1:K:18:ARG:O	1:K:207:PRO:HD3	2.18	0.44
1:L:74:ASP:O	1:L:78:ILE:HG13	2.18	0.44
5:P:315:VAL:HG22	14:P:2103:HOH:O	2.17	0.44
2:C:397:GLU:H	2:C:633:GLN:NE2	2.16	0.43
3:D:260:GLU:HG3	3:D:294:HIS:HE1	1.83	0.43
2:M:943:VAL:HG21	2:M:973:VAL:HG13	2.00	0.43
2:M:1053:LEU:HA	3:N:621:LYS:HD2	2.00	0.43
6:R:4:DT:H2''	6:R:5:DG:C8	2.53	0.43
2:C:1090:LYS:HA	2:C:1090:LYS:HD3	1.85	0.43
2:C:33:ASP:HB2	14:C:1386:HOH:O	2.17	0.43
3:D:561:GLY:HA3	5:F:132:ARG:HD3	2.00	0.43
1:K:83:LYS:NZ	2:M:698:ASP:OD1	2.51	0.43
1:K:97:VAL:HG12	1:K:99:LEU:HD12	1.98	0.43
2:M:23:VAL:HA	2:M:121:MET:SD	2.57	0.43
2:M:937:ASP:OD2	2:M:939:ARG:NH1	2.50	0.43
5:P:172:ARG:O	5:P:176:ILE:HG12	2.17	0.43
3:N:1266:ARG:HD3	7:S:19:DG:H5''	1.99	0.43
2:C:792:VAL:HA	2:C:793:PRO:HD3	1.86	0.43
3:D:367:ILE:HD11	3:D:379:ALA:HB2	2.00	0.43
2:M:170:PRO:HG3	2:M:260:LEU:HD11	1.99	0.43
2:M:432:ARG:HD2	2:M:518:LYS:O	2.18	0.43
2:M:605:LYS:HB2	2:M:612:VAL:HB	2.00	0.43
2:M:802:ARG:HH12	2:M:804:VAL:HG23	1.84	0.43
3:N:43:GLY:H	3:N:46:ASP:HB2	1.82	0.43
1:A:99:LEU:HD21	1:A:122:ILE:HD11	1.99	0.43
2:C:1065:ALA:CB	2:C:1077:PRO:HG3	2.48	0.43
2:C:805:ARG:O	2:C:807:ARG:NH2	2.51	0.43
5:F:88:ILE:HD11	5:F:192:LEU:HD13	2.00	0.43
1:K:90:LEU:HD13	1:K:90:LEU:HA	1.89	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:299:LYS:HB2	2:M:299:LYS:HE3	1.79	0.43
5:P:96:LEU:O	5:P:100:VAL:HG23	2.19	0.43
2:M:335:THR:O	2:M:339:LEU:HG	2.18	0.43
3:N:1274:ILE:HG22	3:N:1324:PRO:HA	2.01	0.43
3:N:1491:THR:HG22	3:N:1495:ILE:HD12	1.99	0.43
5:P:329:TYR:CE2	5:P:333:ILE:HD11	2.52	0.43
2:C:874:LEU:HD23	3:D:1023:MET:SD	2.57	0.43
5:F:325:LYS:HB3	5:F:325:LYS:HE2	1.75	0.43
2:M:797:GLY:O	2:M:829:GLN:NE2	2.52	0.43
5:P:89:GLY:HA3	7:S:7:DG:O6	2.19	0.43
1:A:87:VAL:HG21	1:A:144:VAL:HG21	2.01	0.43
1:B:85:LEU:HG	1:B:87:VAL:HG23	2.01	0.43
4:E:14:ASP:N	4:E:14:ASP:OD2	2.45	0.43
1:K:216:GLU:OE2	1:K:219:ARG:NH2	2.52	0.43
2:M:625:LEU:HB3	2:M:639:GLN:HB2	2.01	0.43
2:M:792:VAL:HA	2:M:793:PRO:HD3	1.86	0.43
3:N:252:ARG:HD2	3:N:301:GLY:O	2.19	0.43
3:N:707:THR:HG23	3:N:712:GLY:HA3	1.99	0.43
3:N:784:ASP:HB2	3:N:939:PHE:HE2	1.84	0.43
2:C:224:GLU:CD	2:C:224:GLU:H	2.21	0.43
2:C:626:ARG:HG3	2:C:629:TYR:CD2	2.53	0.43
3:D:200:ASP:O	3:D:397:LYS:HG2	2.18	0.43
5:F:259:ARG:HD2	14:F:2135:HOH:O	2.19	0.43
2:C:1031:ARG:HG2	6:G:16:DT:H5"	2.01	0.43
1:L:154:GLU:OE1	1:L:154:GLU:N	2.50	0.43
1:L:179:PHE:HB3	1:L:197:LEU:HD13	2.00	0.43
2:M:944:LEU:HA	2:M:944:LEU:HD23	1.86	0.43
3:N:520:LEU:O	3:N:525:ARG:NE	2.50	0.43
1:B:128:HIS:HE1	1:B:131:THR:HG23	1.83	0.43
2:C:884:GLN:O	2:C:888:THR:OG1	2.29	0.43
3:D:185:VAL:N	3:D:201:GLY:O	2.40	0.43
3:D:411:THR:O	5:F:178:ARG:NH1	2.44	0.43
3:D:573:MET:SD	5:F:210:LEU:HB3	2.58	0.43
3:D:966:GLU:O	3:D:969:ARG:HB3	2.18	0.43
3:N:127:LEU:HA	3:N:457:GLY:HA2	2.00	0.43
2:M:1043:TYR:CG	3:N:763:MET:HG2	2.54	0.43
3:D:1018:ASN:HA	3:D:1019:PRO:HD3	1.91	0.43
3:D:1273:VAL:H	3:D:1326:THR:HB	1.83	0.43
3:D:1379:VAL:HG12	3:D:1419:PRO:HA	2.00	0.43
3:D:1450:ALA:HA	3:D:1455:LYS:HE3	2.00	0.43
5:F:326:ASP:OD2	6:G:18:DG:N1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:66:SER:HB2	1:K:75:VAL:HG21	2.00	0.43
3:N:1312:LEU:HD12	3:N:1324:PRO:HB2	2.01	0.43
3:N:654:LYS:O	3:N:658:LEU:HG	2.19	0.43
1:B:176:ARG:HG2	1:B:200:TRP:CE3	2.53	0.42
2:C:92:ALA:HB2	2:C:120:LEU:HD11	2.00	0.42
2:M:470:PRO:HB3	2:M:485:TYR:CE1	2.54	0.42
2:M:704:HIS:CD2	2:M:831:ARG:HD2	2.54	0.42
3:N:180:LYS:HE2	3:N:180:LYS:HB3	1.83	0.42
5:P:282:LEU:HD22	5:P:284:ARG:NH2	2.34	0.42
7:S:18:DC:H2''	7:S:19:DG:O4'	2.19	0.42
2:C:881:ASN:N	2:C:881:ASN:OD1	2.52	0.42
3:D:1420:LEU:HA	3:D:1420:LEU:HD12	1.88	0.42
3:D:1488:ASP:OD1	14:D:2102:HOH:O	2.21	0.42
4:E:13:VAL:HG21	4:E:19:LEU:HB2	2.01	0.42
5:F:172:ARG:O	5:F:176:ILE:HG12	2.19	0.42
5:F:226:LYS:HE3	5:F:226:LYS:HB3	1.74	0.42
3:N:236:TYR:CZ	3:N:242:LEU:HD12	2.54	0.42
3:N:95:LEU:HA	3:N:551:ASN:HD21	1.84	0.42
1:A:54:THR:HG21	1:A:145:ASP:HB2	2.00	0.42
2:C:916:GLU:O	2:C:920:GLN:HG3	2.18	0.42
2:M:332:ARG:HB3	2:M:466:PHE:CD2	2.54	0.42
2:M:707:ARG:NH1	14:M:1315:HOH:O	2.52	0.42
3:N:285:PRO:HD2	3:N:288:MET:SD	2.58	0.42
1:B:48:ILE:HA	1:B:49:PRO:HD3	1.80	0.42
2:C:946:ARG:HG3	14:C:1335:HOH:O	2.19	0.42
2:C:984:GLU:OE2	3:D:791:TYR:OH	2.30	0.42
2:C:359:MET:HG2	2:C:372:LEU:HD22	2.01	0.42
3:D:181:ASP:HB2	3:D:205:TYR:CD1	2.53	0.42
3:D:474:GLU:HG3	3:D:496:LEU:HD11	2.02	0.42
3:D:68:PHE:O	3:D:71:LYS:HB3	2.19	0.42
3:D:899:LEU:HD22	3:D:917:GLN:HB3	2.01	0.42
2:M:168:ARG:HH12	2:M:345:ARG:HD3	1.85	0.42
1:A:26:GLU:HB3	1:A:194:LYS:HG3	2.01	0.42
2:C:328:LEU:HA	2:C:328:LEU:HD23	1.87	0.42
3:D:1485:GLN:O	4:E:75:PHE:HA	2.20	0.42
3:D:241:ILE:HD11	3:D:310:LEU:HB3	2.02	0.42
2:M:328:LEU:HD23	2:M:328:LEU:HA	1.73	0.42
2:M:642:ARG:HG3	2:M:654:LEU:HD21	2.02	0.42
1:B:52:ALA:HB2	1:B:170:VAL:O	2.20	0.42
2:C:212:GLY:HA2	2:C:218:VAL:HG11	2.00	0.42
2:C:642:ARG:HA	2:C:642:ARG:HD3	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:922:PHE:CE2	2:C:964:LYS:HB2	2.55	0.42
3:D:1461:GLY:O	3:D:1465:ASN:ND2	2.51	0.42
3:D:612:GLY:O	3:D:616:GLN:HB3	2.19	0.42
3:D:654:LYS:O	3:D:658:LEU:HG	2.19	0.42
2:M:705:ILE:HG12	2:M:828:ALA:HB2	2.01	0.42
3:N:472:ALA:O	3:N:476:GLU:HG2	2.20	0.42
7:S:8:DG:H2''	7:S:9:DG:C8	2.54	0.42
2:C:575:GLN:OE1	2:C:670:GLN:HG3	2.20	0.42
3:D:472:ALA:O	3:D:476:GLU:HG2	2.20	0.42
3:D:540:LEU:HD23	3:D:540:LEU:HA	1.92	0.42
3:D:659:LYS:HD2	3:D:659:LYS:HA	1.90	0.42
3:D:971:LEU:HA	3:D:971:LEU:HD22	1.83	0.42
4:E:45:ARG:HA	4:E:46:PRO:HD3	1.89	0.42
2:M:398:THR:OG1	2:M:633:GLN:HG2	2.20	0.42
3:N:1256:LEU:O	3:N:1260:ILE:HG13	2.19	0.42
3:N:1267:ARG:HA	3:N:1268:PRO:HD3	1.87	0.42
5:P:265:VAL:HG12	5:P:269:ASN:ND2	2.34	0.42
3:D:1498:ALA:O	3:D:1501:GLU:HB3	2.20	0.42
1:L:73:GLU:HB3	1:L:77:GLU:HB3	2.01	0.42
2:M:708:TYR:HB3	2:M:790:LEU:HD21	2.02	0.42
3:N:637:LEU:HD13	3:N:642:CYS:HA	2.00	0.42
1:A:133:GLU:HG3	2:C:645:VAL:HG21	2.01	0.42
3:D:140:ALA:HA	3:D:450:TYR:CD2	2.55	0.42
3:D:159:ARG:NH2	14:D:2123:HOH:O	2.52	0.42
3:D:38:LYS:HD3	3:D:38:LYS:HA	1.68	0.42
3:D:711:LEU:HD13	3:D:778:LEU:HD23	2.02	0.42
1:K:218:LEU:HD23	1:L:222:LEU:HD21	2.02	0.42
2:M:160:ALA:HB2	2:M:310:LEU:HD13	2.01	0.42
3:N:1168:MET:HE3	3:N:1168:MET:HA	2.02	0.42
3:D:1137:ARG:O	3:D:1141:GLU:HG3	2.19	0.41
3:D:970:LYS:O	3:D:974:ILE:HG12	2.19	0.41
5:F:333:ILE:HA	5:F:334:PRO:HD3	1.86	0.41
2:M:249:LYS:HB2	2:M:249:LYS:HE3	1.70	0.41
2:M:29:ALA:O	2:M:44:ILE:HG22	2.20	0.41
2:M:674:VAL:O	2:M:989:VAL:HA	2.20	0.41
3:N:1130:ARG:NE	3:N:1130:ARG:O	2.53	0.41
3:N:1292:VAL:HG23	3:N:1305:LEU:HD21	2.02	0.41
3:N:684:LYS:HE2	3:N:684:LYS:HB3	1.79	0.41
2:C:43:GLY:O	2:C:46:ALA:HB3	2.20	0.41
3:D:1362:LYS:HE2	3:D:1362:LYS:HB2	1.89	0.41
5:F:153:PRO:HA	5:F:156:VAL:HG22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:80:PRO:HB2	5:F:210:LEU:HD11	2.02	0.41
2:M:431:HIS:HB3	2:M:434:HIS:ND1	2.36	0.41
3:N:792:ILE:HD13	3:N:941:PHE:CE1	2.54	0.41
1:B:30:ARG:NH2	2:C:854:PRO:HB3	2.35	0.41
3:D:135:LEU:HD23	3:D:455:ARG:HH21	1.84	0.41
3:D:929:ARG:HD3	14:D:2240:HOH:O	2.19	0.41
5:F:326:ASP:N	5:F:326:ASP:OD1	2.53	0.41
2:M:195:LEU:HG	2:M:238:LEU:HD12	2.02	0.41
3:N:1065:LEU:HD23	3:N:1070:TYR:HA	2.03	0.41
6:R:11:DG:H2''	6:R:12:DT:H5'	2.03	0.41
3:D:879:ARG:HD3	3:D:902:LEU:O	2.21	0.41
3:D:97:THR:HG21	3:D:571:LYS:HG2	2.02	0.41
2:M:165:LEU:HD22	2:M:166:PRO:HD2	2.02	0.41
2:M:709:GLU:OE2	2:M:824:ARG:NH1	2.53	0.41
3:N:115:LEU:HA	3:N:115:LEU:HD23	1.95	0.41
3:N:66:GLN:HB2	3:N:66:GLN:HE21	1.57	0.41
3:N:784:ASP:HB2	3:N:939:PHE:CE2	2.55	0.41
1:B:106:PRO:HA	1:B:132:LEU:O	2.21	0.41
2:C:160:ALA:HB3	2:C:174:LEU:HB2	2.01	0.41
3:D:1307:LYS:H	3:D:1307:LYS:HG3	1.70	0.41
3:D:353:VAL:HG11	3:D:387:LEU:HD11	2.03	0.41
1:K:36:LEU:HD23	1:K:36:LEU:HA	1.85	0.41
2:M:164:PRO:HA	2:M:269:LEU:HD23	2.02	0.41
2:M:290:LEU:HB2	14:M:1301:HOH:O	2.19	0.41
2:M:141:HIS:CE1	2:M:334:ARG:HD2	2.56	0.41
3:N:1487:VAL:HG22	3:N:1491:THR:HB	2.01	0.41
3:N:544:TYR:O	3:N:548:ILE:HG13	2.21	0.41
3:N:54:LYS:NZ	3:N:54:LYS:HB3	2.36	0.41
3:N:961:LYS:HB2	3:N:961:LYS:HE3	1.90	0.41
4:O:40:LEU:HG	4:O:67:GLU:HG2	2.02	0.41
2:C:628:PHE:N	2:C:638:ASP:HB3	2.29	0.41
3:D:1264:GLU:OE2	3:D:1425:THR:OG1	2.38	0.41
3:D:800:LYS:HE2	3:D:819:GLY:O	2.21	0.41
5:F:120:THR:HG22	5:F:122:LEU:HD13	2.02	0.41
1:K:41:ARG:HA	1:K:177:VAL:HG11	2.03	0.41
1:K:20:TYR:OH	1:K:198:ARG:HD2	2.20	0.41
2:M:1081:VAL:HA	2:M:1082:PRO:HD2	1.87	0.41
3:N:658:LEU:HD23	3:N:661:MET:CE	2.50	0.41
3:N:899:LEU:HD22	3:N:917:GLN:HB3	2.01	0.41
1:B:57:TYR:CE1	1:B:163:ASN:HB2	2.56	0.41
1:L:115:LEU:HA	1:L:116:PRO:HD3	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:175:ARG:N	1:L:200:TRP:O	2.49	0.41
2:M:66:LEU:HD22	2:M:355:VAL:HG11	2.03	0.41
5:P:93:LEU:HD11	7:S:6:DT:H2"	2.02	0.41
3:D:1150:ALA:HB3	3:D:1187:PRO:HB2	2.02	0.41
3:D:149:LYS:HE3	3:D:149:LYS:HB3	1.91	0.41
1:K:39:PRO:CG	1:L:39:PRO:HG3	2.50	0.41
1:L:101:LEU:HD11	1:L:113:ASP:HB2	2.01	0.41
2:M:286:SER:OG	2:M:292:ARG:HD3	2.19	0.41
3:N:633:VAL:C	3:N:635:PRO:HD3	2.41	0.41
3:N:841:TYR:HB2	3:N:864:VAL:CG2	2.51	0.41
2:M:778:PHE:CZ	5:P:419:ARG:HA	2.56	0.41
1:A:218:LEU:HG	1:B:222:LEU:HD11	2.03	0.41
1:A:9:PRO:HB3	1:A:27:PRO:O	2.20	0.41
2:C:12:VAL:HG21	2:C:472:ARG:HD3	2.03	0.41
2:C:413:LEU:HD12	2:C:452:ILE:HD11	2.01	0.41
3:D:168:THR:OG1	3:D:394:LEU:HD13	2.20	0.41
4:E:30:LEU:HD23	4:E:30:LEU:HA	1.83	0.41
4:E:31:LEU:HA	4:E:31:LEU:HD23	1.76	0.41
5:F:101:GLU:HG2	5:F:105:LYS:HE2	2.02	0.41
5:F:416:ARG:O	5:F:416:ARG:HD3	2.21	0.41
1:K:48:ILE:HA	1:K:49:PRO:HD3	1.93	0.41
1:L:132:LEU:HD21	1:L:138:LEU:HB2	2.03	0.41
1:L:222:LEU:HD23	1:L:222:LEU:HA	1.91	0.41
2:M:420:ARG:C	2:M:422:ARG:H	2.24	0.41
2:M:599:GLU:HG3	2:M:600:ASP:H	1.86	0.41
3:N:438:ASP:OD1	3:N:441:ARG:NH2	2.53	0.41
2:C:76:PRO:HG3	2:C:120:LEU:CD1	2.50	0.41
3:D:1144:LEU:HA	3:D:1144:LEU:HD23	1.86	0.41
3:D:372:ASP:HB3	3:D:374:GLU:OE2	2.21	0.41
2:M:13:ILE:HG13	2:M:458:TYR:HE2	1.84	0.41
1:K:70:GLY:N	2:M:607:ASP:OD1	2.54	0.41
3:N:1373:ARG:HD3	14:N:2204:HOH:O	2.21	0.41
3:N:935:LYS:HE2	3:N:935:LYS:HB3	1.94	0.41
1:A:101:LEU:HB2	1:A:114:PHE:CD2	2.56	0.41
2:C:195:LEU:O	2:C:199:VAL:HG23	2.20	0.41
2:C:684:PHE:HB3	3:D:633:VAL:HG21	2.03	0.41
3:D:844:ALA:O	3:D:867:ARG:HB3	2.21	0.41
1:K:89:PHE:HE2	1:K:95:GLN:O	2.03	0.41
2:M:247:PRO:HA	2:M:248:PRO:HD3	1.75	0.41
3:N:709:HIS:ND1	3:N:1231:GLU:HG3	2.36	0.41
1:A:133:GLU:HG2	1:A:134:GLU:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:PHE:HE1	1:B:47:SER:HG	1.68	0.40
2:M:274:ARG:HH12	2:M:286:SER:C	2.24	0.40
1:K:70:GLY:H	2:M:607:ASP:CG	2.23	0.40
2:M:764:GLU:HG3	2:M:764:GLU:H	1.53	0.40
2:M:944:LEU:HD11	2:M:963:LEU:HG	2.03	0.40
3:N:880:ILE:HD13	3:N:880:ILE:HA	1.98	0.40
5:P:338:LEU:HA	5:P:339:PRO:HD3	1.92	0.40
1:B:150:TYR:CE1	1:B:170:VAL:HG22	2.56	0.40
1:B:80:LEU:O	1:B:83:LYS:HB2	2.21	0.40
2:C:599:GLU:HG3	2:C:600:ASP:H	1.86	0.40
2:C:76:PRO:HA	2:C:77:PRO:HD2	1.88	0.40
3:D:255:GLU:HG3	3:D:280:ALA:HB2	2.03	0.40
5:F:120:THR:HG21	5:F:122:LEU:HD22	2.03	0.40
5:F:152:ASP:HB2	5:F:153:PRO:HD2	2.03	0.40
3:N:1378:TYR:CZ	3:N:1430:SER:HB2	2.57	0.40
3:N:708:LEU:HA	3:N:708:LEU:HD23	1.85	0.40
5:P:237:THR:OG1	7:S:4:DA:H8	2.03	0.40
1:A:211:LEU:O	1:A:215:VAL:HG23	2.21	0.40
2:C:380:ALA:O	2:C:384:GLU:HB3	2.21	0.40
2:C:944:LEU:HD23	2:C:944:LEU:HA	1.95	0.40
3:D:1112:CYS:SG	3:D:1114:THR:HG22	2.61	0.40
1:K:45:LEU:HD23	1:K:45:LEU:HA	1.90	0.40
2:M:1065:ALA:CB	2:M:1077:PRO:HG3	2.51	0.40
3:N:1379:VAL:HG21	3:N:1400:VAL:HG11	2.03	0.40
2:M:1071:ILE:HD12	3:N:670:VAL:HG11	2.03	0.40
3:N:988:ARG:O	3:N:992:ILE:HG13	2.22	0.40
4:O:83:ASP:O	4:O:87:LYS:HG2	2.21	0.40
4:O:9:LEU:HA	4:O:9:LEU:HD23	1.93	0.40
1:A:11:PHE:O	1:B:228:PRO:HA	2.21	0.40
1:B:115:LEU:HA	1:B:116:PRO:HD3	1.91	0.40
2:C:168:ARG:O	2:C:267:TYR:HA	2.20	0.40
3:D:814:ALA:O	3:D:818:ARG:HG3	2.21	0.40
5:F:148:LYS:HE3	5:F:148:LYS:HB2	1.80	0.40
5:F:362:SER:OG	5:F:365:GLU:HG2	2.21	0.40
1:K:64:GLU:HG2	1:K:76:VAL:HG22	2.02	0.40
1:L:143:ARG:HG2	1:L:158:ILE:HD11	2.03	0.40
2:M:493:ARG:NH1	2:M:494:TYR:OH	2.54	0.40
2:M:886:LEU:HD21	3:N:951:ILE:HG12	2.03	0.40
3:N:468:LEU:HA	3:N:468:LEU:HD23	1.89	0.40
3:N:677:LEU:HA	3:N:683:ILE:HD11	2.03	0.40
3:N:834:THR:OG1	3:N:835:SER:N	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:140:ARG:HB2	5:P:142:ARG:HD3	2.02	0.40
5:P:338:LEU:HA	5:P:338:LEU:HD23	1.98	0.40
5:P:416:ARG:O	5:P:419:ARG:HG2	2.21	0.40
3:N:671:LYS:NZ	5:P:421:PHE:HA	2.37	0.40
2:C:631:SER:HB3	2:C:637:LEU:HD13	2.02	0.40
3:D:192:ALA:HB1	3:D:193:PRO:HD2	2.02	0.40
3:D:260:GLU:HG3	3:D:294:HIS:CE1	2.57	0.40
3:D:685:ASP:HA	3:D:688:TRP:HD1	1.87	0.40
2:M:1102:LEU:HD23	2:M:1108:PRO:HA	2.03	0.40
2:M:775:ARG:CZ	2:M:782:ALA:HB2	2.52	0.40
3:N:1366:LYS:O	3:N:1370:ILE:HG12	2.22	0.40
3:N:1383:ASP:HA	3:N:1384:PRO:HD3	1.80	0.40
3:N:1490:LYS:HB2	3:N:1490:LYS:HE3	1.88	0.40
3:N:574:LEU:O	3:N:578:VAL:HG23	2.22	0.40
3:N:864:VAL:HG13	3:N:865:THR:N	2.37	0.40
4:O:41:GLU:O	4:O:45:ARG:HG3	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:327:GLU:OE2	5:P:263:HIS:NE2[2_545]	2.16	0.04

## 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	227/315 (72%)	224 (99%)	3 (1%)	0	100	100
1	B	218/315 (69%)	214 (98%)	4 (2%)	0	100	100
1	K	226/315 (72%)	221 (98%)	5 (2%)	0	100	100
1	L	218/315 (69%)	213 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	1102/1119 (98%)	1076 (98%)	26 (2%)	0	100	100
2	M	1083/1119 (97%)	1050 (97%)	33 (3%)	0	100	100
3	D	1481/1524 (97%)	1452 (98%)	29 (2%)	0	100	100
3	N	1479/1524 (97%)	1449 (98%)	28 (2%)	2 (0%)	56	90
4	E	92/99 (93%)	90 (98%)	2 (2%)	0	100	100
4	O	92/99 (93%)	90 (98%)	2 (2%)	0	100	100
5	F	344/443 (78%)	339 (98%)	5 (2%)	0	100	100
5	P	310/443 (70%)	304 (98%)	6 (2%)	0	100	100
All	All	6872/7630 (90%)	6722 (98%)	148 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	N	1131	SER
3	N	530	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	199/273 (73%)	192 (96%)	7 (4%)	43	80
1	B	195/273 (71%)	189 (97%)	6 (3%)	47	83
1	K	199/273 (73%)	193 (97%)	6 (3%)	48	83
1	L	195/273 (71%)	189 (97%)	6 (3%)	47	83
2	C	933/941 (99%)	899 (96%)	34 (4%)	42	79
2	M	917/941 (97%)	876 (96%)	41 (4%)	34	74
3	D	1252/1279 (98%)	1196 (96%)	56 (4%)	34	74
3	N	1251/1279 (98%)	1195 (96%)	56 (4%)	34	74
4	E	82/88 (93%)	79 (96%)	3 (4%)	41	79
4	O	82/88 (93%)	77 (94%)	5 (6%)	23	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	F	301/388 (78%)	293 (97%)	8 (3%)	52 85
5	P	277/388 (71%)	258 (93%)	19 (7%)	19 56
All	All	5883/6484 (91%)	5636 (96%)	247 (4%)	36 76

All (247) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	12	THR
1	A	66	SER
1	A	102	LYS
1	A	126	ASP
1	A	205	VAL
1	A	229	GLN
1	B	10	VAL
1	B	15	THR
1	B	126	ASP
1	B	154	GLU
1	B	184	THR
1	B	197	LEU
2	C	87	ASP
2	C	141	HIS
2	C	210	GLU
2	C	211	LEU
2	C	217	LEU
2	C	222	MET
2	C	246	ASP
2	C	250	ARG
2	C	261	ILE
2	C	284	ARG
2	C	285	LEU
2	C	358	ARG
2	C	360	LEU
2	C	361	MET
2	C	367	LEU
2	C	384	GLU
2	C	409	ARG
2	C	421	GLU
2	C	429	ASP
2	C	454	SER
2	C	489	THR

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Mol	Chain	Res	Type
2	C	610	ARG
2	C	617	ASP
2	C	670	GLN
2	C	738	ASP
2	C	766	GLU
2	C	807	ARG
2	C	815	LEU
2	C	816	LYS
2	C	939	ARG
2	C	952	LEU
2	C	978	ARG
2	C	1080	SER
2	C	1117	SER
3	D	35	ARG
3	D	65	ARG
3	D	67	ARG
3	D	71	LYS
3	D	115	LEU
3	D	161	LEU
3	D	178	LEU
3	D	191	LEU
3	D	231	VAL
3	D	241	ILE
3	D	273	ARG
3	D	311	LEU
3	D	312	ARG
3	D	346	ARG
3	D	374	GLU
3	D	387	LEU
3	D	407	VAL
3	D	527	MET
3	D	611	GLN
3	D	618	LEU
3	D	632	VAL
3	D	681	ARG
3	D	687	VAL
3	D	709	HIS
3	D	710	ARG
3	D	754	PHE
3	D	778	LEU
3	D	784	ASP
3	D	808	THR

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Mol	Chain	Res	Type
3	D	864	VAL
3	D	894	LYS
3	D	904	VAL
3	D	907	GLU
3	D	949	ILE
3	D	956	ILE
3	D	971	LEU
3	D	984	THR
3	D	986	ARG
3	D	1001	GLU
3	D	1041	LEU
3	D	1067	VAL
3	D	1129	THR
3	D	1132	LEU
3	D	1152	GLU
3	D	1155	VAL
3	D	1188	VAL
3	D	1208	ASP
3	D	1219	GLU
3	D	1253	THR
3	D	1267	ARG
3	D	1280	VAL
3	D	1290	LEU
3	D	1295	GLU
3	D	1307	LYS
3	D	1430	SER
3	D	1486	VAL
4	E	51	LEU
4	E	55	PHE
4	E	92	LEU
5	F	88	ILE
5	F	150	THR
5	F	205	ARG
5	F	279	GLN
5	F	324	GLU
5	F	416	ARG
5	F	417	LYS
5	F	420	ASP
1	K	6	LEU
1	K	10	VAL
1	K	74	ASP
1	K	96	THR

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Mol	Chain	Res	Type
1	K	126	ASP
1	K	196	THR
1	L	67	THR
1	L	96	THR
1	L	101	LEU
1	L	126	ASP
1	L	145	ASP
1	L	146	ARG
2	M	20	GLU
2	M	27	ARG
2	M	44	ILE
2	M	49	ARG
2	M	51	THR
2	M	54	ILE
2	M	64	LEU
2	M	113	VAL
2	M	141	HIS
2	M	149	THR
2	M	188	LYS
2	M	194	VAL
2	M	204	GLN
2	M	206	THR
2	M	210	GLU
2	M	214	TYR
2	M	216	GLU
2	M	221	LEU
2	M	284	ARG
2	M	294	GLU
2	M	358	ARG
2	M	388	ARG
2	M	394	PHE
2	M	402	SER
2	M	454	SER
2	M	504	GLU
2	M	566	THR
2	M	610	ARG
2	M	640	ARG
2	M	670	GLN
2	M	698	ASP
2	M	730	SER
2	M	768	THR
2	M	771	GLU

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Mol	Chain	Res	Type
2	M	781	LYS
2	M	807	ARG
2	M	808	ARG
2	M	929	ARG
2	M	939	ARG
2	M	952	LEU
2	M	978	ARG
3	N	36	THR
3	N	54	LYS
3	N	66	GLN
3	N	106	LYS
3	N	130	SER
3	N	145	VAL
3	N	176	ASP
3	N	191	LEU
3	N	196	VAL
3	N	249	TYR
3	N	270	LEU
3	N	310	LEU
3	N	315	ARG
3	N	340	THR
3	N	343	LYS
3	N	367	ILE
3	N	374	GLU
3	N	378	ILE
3	N	400	VAL
3	N	420	VAL
3	N	421	LEU
3	N	430	ASP
3	N	601	ARG
3	N	618	LEU
3	N	628	ARG
3	N	632	VAL
3	N	650	LEU
3	N	709	HIS
3	N	724	GLN
3	N	725	SER
3	N	753	SER
3	N	754	PHE
3	N	810	GLU
3	N	864	VAL
3	N	904	VAL

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Mol	Chain	Res	Type
3	N	971	LEU
3	N	979	GLU
3	N	986	ARG
3	N	1001	GLU
3	N	1005	GLN
3	N	1039	CYS
3	N	1042	ARG
3	N	1096	ARG
3	N	1130	ARG
3	N	1132	LEU
3	N	1154	GLU
3	N	1282	ARG
3	N	1284	GLU
3	N	1299	PHE
3	N	1305	LEU
3	N	1307	LYS
3	N	1314	LYS
3	N	1487	VAL
3	N	1493	LYS
3	N	1497	GLU
3	N	1500	LYS
4	O	51	LEU
4	O	80	VAL
4	O	82	GLU
4	O	83	ASP
4	O	93	TYR
5	P	95	THR
5	P	140	ARG
5	P	142	ARG
5	P	149	GLU
5	P	150	THR
5	P	151	LEU
5	P	170	HIS
5	P	186	HIS
5	P	271	LEU
5	P	277	GLN
5	P	315	VAL
5	P	319	THR
5	P	321	ILE
5	P	346	THR
5	P	367	MET
5	P	396	ARG

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Mol	Chain	Res	Type
5	P	402	ASN
5	P	403	LYS
5	P	419	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	99	GLN
2	C	102	HIS
2	C	390	GLN
2	C	633	GLN
2	C	1047	HIS
2	C	1107	ASN
3	D	66	GLN
3	D	294	HIS
3	D	762	GLN
3	D	994	GLN
3	D	1046	GLN
3	D	1184	GLN
3	D	1195	GLN
3	D	1359	GLN
3	D	1442	ASN
5	F	83	GLN
5	F	175	HIS
1	K	63	HIS
1	K	212	ASN
1	K	213	GLN
2	M	31	GLN
2	M	204	GLN
2	M	390	GLN
3	N	66	GLN
3	N	724	GLN
3	N	1046	GLN
3	N	1116	ASN
3	N	1124	GLN
3	N	1172	HIS
3	N	1195	GLN
5	P	83	GLN
5	P	269	ASN
5	P	280	GLN
5	P	347	GLN



### 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 20 ligands modelled in this entry, 14 are monoatomic - leaving 6 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
10	C	D	2005	8,12	14,21,22	0.72	0	18,30,33	0.55	0
11	CTP	D	2006	8	6,8,30	1.73	1 (16%)	6,13,47	0.71	0
12	NAD	D	2008	10	42,48,48	2.05	11 (26%)	46,73,73	2.32	9 (19%)
11	CTP	M	1201	8	6,8,30	1.19	1 (16%)	6,13,47	0.52	0
10	C	N	2005	8	14,21,22	0.74	0	18,30,33	0.53	0
13	A	R	101	-	22,25,25	2.08	7 (31%)	22,38,38	2.50	2 (9%)

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
10	C	D	2005	8,12	-	0/3/25/26	0/2/2/2
11	CTP	D	2006	8	-	0/6/6/38	0/0/0/2
12	NAD	D	2008	10	-	0/22/62/62	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CTP	M	1201	8	-	0/6/6/38	0/0/0/2
10	C	N	2005	8	-	0/3/25/26	0/2/2/2
13	A	R	101	-	-	0/6/26/26	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	2008	NAD	O2D-C2D	-2.84	1.36	1.43
12	D	2008	NAD	O2B-C2B	-2.50	1.37	1.43
13	R	101	A	O2'-C2'	-2.44	1.37	1.43
12	D	2008	NAD	C2B-C3B	-2.18	1.47	1.53
12	D	2008	NAD	O3D-C3D	-2.17	1.37	1.43
13	R	101	A	C2'-C3'	-2.12	1.47	1.53
12	D	2008	NAD	C2D-C3D	-2.03	1.48	1.53
13	R	101	A	O3'-C3'	-2.02	1.38	1.43
12	D	2008	NAD	C6A-N6A	2.31	1.43	1.34
11	M	1201	CTP	PA-O5'	2.33	1.62	1.54
13	R	101	A	C6-N6	2.38	1.43	1.34
12	D	2008	NAD	C2A-N1A	3.26	1.40	1.33
13	R	101	A	C2-N1	3.37	1.40	1.33
11	D	2006	CTP	PA-O1A	3.74	1.62	1.50
12	D	2008	NAD	C2A-N3A	4.21	1.39	1.32
13	R	101	A	C2-N3	4.21	1.39	1.32
12	D	2008	NAD	O4D-C1D	5.09	1.48	1.41
12	D	2008	NAD	O4B-C1B	5.42	1.49	1.41
13	R	101	A	O4'-C1'	5.53	1.49	1.41
12	D	2008	NAD	C7N-N7N	5.58	1.44	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	R	101	A	N3-C2-N1	-9.49	121.41	128.87
12	D	2008	NAD	N3A-C2A-N1A	-9.42	121.47	128.87
12	D	2008	NAD	C4D-O4D-C1D	-3.21	106.24	109.64
12	D	2008	NAD	O7N-C7N-N7N	-2.50	119.02	122.58
12	D	2008	NAD	C4B-O4B-C1B	-2.20	107.32	109.64
12	D	2008	NAD	C2D-C1D-N1N	2.04	117.52	113.53
12	D	2008	NAD	C2D-C3D-C4D	2.38	107.50	102.64
12	D	2008	NAD	C3N-C7N-N7N	3.25	121.49	117.82
12	D	2008	NAD	O4B-C1B-N9A	5.44	118.37	108.11
13	R	101	A	O4'-C1'-N9	5.58	118.65	108.11
12	D	2008	NAD	O4D-C1D-N1N	8.38	117.16	108.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	D	2008	NAD	1	0
10	N	2005	C	2	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	229/315 (72%)	-0.51	1 (0%) 93 80	7, 21, 48, 79	1 (0%)
1	B	222/315 (70%)	-0.44	0 100 100	6, 31, 64, 81	0
1	K	228/315 (72%)	-0.38	0 100 100	10, 31, 57, 71	1 (0%)
1	L	222/315 (70%)	-0.40	0 100 100	12, 36, 73, 103	0
2	C	1108/1119 (99%)	-0.46	7 (0%) 90 73	0, 14, 62, 89	3 (0%)
2	M	1091/1119 (97%)	-0.12	33 (3%) 54 25	1, 39, 97, 116	2 (0%)
3	D	1485/1524 (97%)	-0.36	7 (0%) 91 76	0, 18, 68, 103	4 (0%)
3	N	1483/1524 (97%)	-0.30	14 (0%) 85 64	0, 24, 77, 106	4 (0%)
4	E	94/99 (94%)	-0.56	1 (1%) 82 58	1, 13, 49, 67	0
4	O	94/99 (94%)	-0.42	0 100 100	4, 23, 62, 71	0
5	F	346/443 (78%)	-0.43	1 (0%) 94 84	3, 26, 68, 84	0
5	P	316/443 (71%)	-0.20	5 (1%) 74 47	17, 46, 91, 109	0
6	G	16/19 (84%)	-0.20	0 100 100	16, 48, 112, 117	0
6	R	16/19 (84%)	-0.12	0 100 100	39, 65, 115, 122	0
7	H	21/27 (77%)	-0.20	1 (4%) 34 14	19, 56, 108, 124	0
7	S	21/27 (77%)	0.03	1 (4%) 34 14	33, 84, 121, 144	0
All	All	6992/7722 (90%)	-0.33	71 (1%) 84 60	0, 26, 78, 144	15 (0%)

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	188	LYS	5.1
2	M	200	LEU	4.5
2	M	196	LEU	4.5
2	M	63	GLY	3.8
2	M	368	THR	3.8

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Mol	Chain	Res	Type	RSRZ
2	M	765	SER	3.6
2	M	217	LEU	3.4
2	M	207	LEU	3.4
2	C	219	GLN	3.2
2	M	228	ALA	3.1
2	C	63	GLY	3.1
2	M	199	VAL	3.1
2	M	202	TYR	3.0
2	M	258	TYR	2.9
2	C	104	ASP	2.8
2	M	358	ARG	2.7
2	M	181	VAL	2.7
5	P	410	TYR	2.7
2	M	52	PHE	2.6
3	D	1130	ARG	2.6
3	N	191	LEU	2.6
3	D	241	ILE	2.6
2	C	105	THR	2.6
3	D	1499	ARG	2.6
4	E	51	LEU	2.6
2	M	179	ASN	2.6
3	N	307	ALA	2.5
2	M	762	LYS	2.5
2	M	371	LYS	2.5
2	M	769	PRO	2.5
2	C	205	GLU	2.5
3	N	311	LEU	2.4
2	M	295	ASP	2.4
3	N	378	ILE	2.4
3	N	424	GLY	2.4
2	M	226	VAL	2.3
3	N	308	LYS	2.3
3	N	345	TYR	2.3
3	N	367	ILE	2.3
2	M	246	ASP	2.3
3	N	1499	ARG	2.3
1	A	231	ALA	2.3
5	F	423	ASP	2.3
3	N	316	GLN	2.3
3	D	219	GLU	2.3
2	M	242	LEU	2.3
3	N	1130	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
2	M	111	ASP	2.2
3	D	1502	ALA	2.2
7	H	25	DA	2.2
2	M	296	GLY	2.2
5	P	397	ILE	2.2
5	P	406	ARG	2.1
2	M	208	ALA	2.1
3	N	309	GLY	2.1
2	M	354	GLY	2.1
3	D	1405	GLU	2.1
2	M	344	PHE	2.1
2	M	65	VAL	2.1
2	M	770	GLU	2.1
2	M	782	ALA	2.1
5	P	407	LYS	2.1
2	C	106	GLY	2.1
2	M	259	GLY	2.1
2	M	372	LEU	2.0
2	C	366	SER	2.0
3	N	1127	GLU	2.0
3	N	802	ALA	2.0
7	S	25	DA	2.0
3	D	1131	SER	2.0
5	P	369	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, 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( $\text{\AA}^2$ )	Q<0.9
13	A	R	101	23/23	0.83	0.25	2.88	37,54,63,83	23
10	C	N	2005	20/21	0.88	0.23	1.69	22,46,53,59	20
12	NAD	D	2008	44/44	0.89	0.24	1.64	15,34,53,67	44
11	CTP	M	1201	9/29	0.89	0.20	1.43	25,52,69,73	0
11	CTP	D	2006	9/29	0.91	0.21	1.30	21,41,62,80	0
10	C	D	2005	20/21	0.94	0.18	0.17	6,19,38,47	20
8	MG	P	2001	1/1	0.92	0.24	-0.22	51,51,51,51	0
9	ZN	D	2001	1/1	1.00	0.14	-0.36	5,5,5,5	0
8	MG	D	2004	1/1	0.99	0.17	-0.36	15,15,15,15	0
9	ZN	N	2001	1/1	1.00	0.15	-1.11	7,7,7,7	0
9	ZN	N	2002	1/1	0.96	0.07	-1.71	89,89,89,89	0
9	ZN	D	2002	1/1	0.99	0.05	-2.28	40,40,40,40	0
8	MG	L	2001	1/1	0.93	0.10	-3.06	41,41,41,41	0
8	MG	N	2004	1/1	0.98	0.06	-3.16	27,27,27,27	0
8	MG	F	2001	1/1	0.93	0.05	-3.17	25,25,25,25	0
8	MG	D	2007	1/1	0.94	0.33	-	28,28,28,28	0
8	MG	N	2006	1/1	0.94	0.28	-	32,32,32,32	0
8	MG	N	2003	1/1	0.93	0.26	-	6,6,6,6	0
8	MG	D	2003	1/1	0.88	0.23	-	1,1,1,1	0
8	MG	B	2001	1/1	0.92	0.20	-	17,17,17,17	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.