



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 11:44 pm BST

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

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

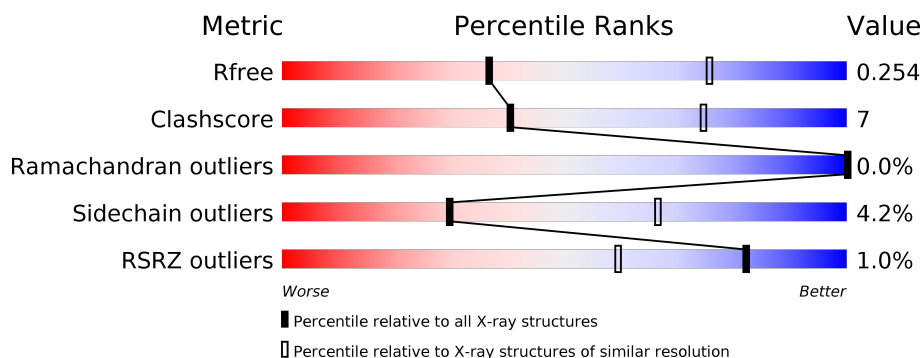
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

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

## 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			

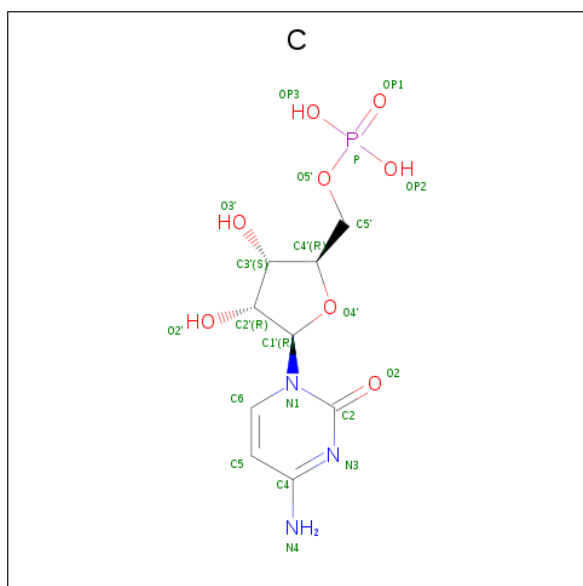
- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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).

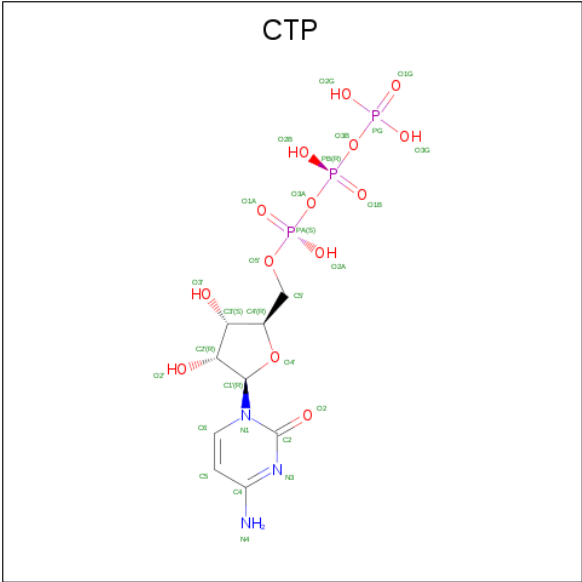
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	D	2	Total	Zn	0	0
			2	2		
9	N	2	Total	Zn	0	0
			2	2		

- 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).



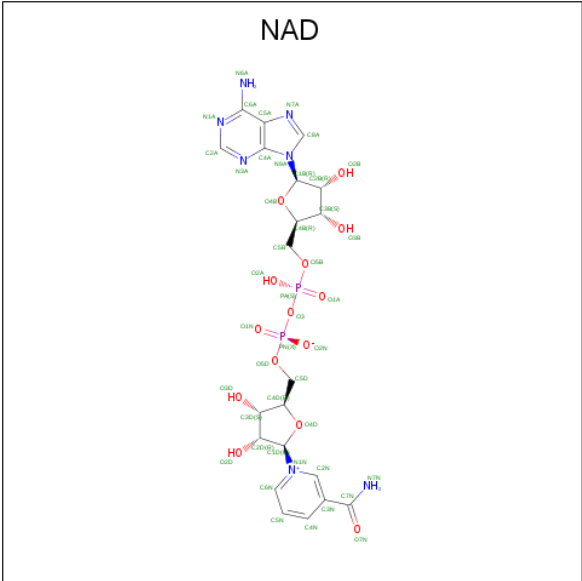
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	D	1	Total	C	N	O	P	0	0
			20	9	3	7	1		
10	N	1	Total	C	N	O	P	0	0
			20	9	3	7	1		

- 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	O	P		0	0
			9	7	2			
11	M	1	Total	O	P		0	0
			9	7	2			

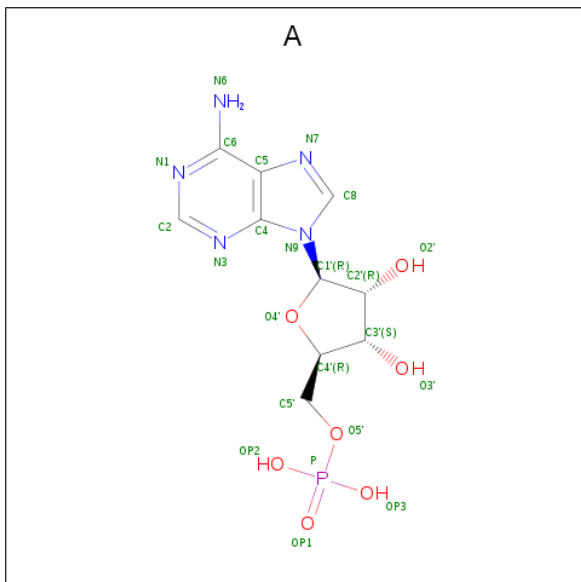
- Molecule 12 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



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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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

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

[illegible]

Chain B:

Residue	Category
LEU	Grey
GLY	Grey
LEU	Grey
SER	Grey
THR	Green
ARG	Green
VAL	Green
LEU	Green
HIS	Yellow
SER	Yellow
LEU	Yellow
LYS	Yellow
GLU	Yellow
GLY	Yellow
GLU	Yellow
ILE	Yellow
SER	Yellow
VAL	Yellow
ARG	Yellow
ALA	Yellow
LEU	Yellow
ALA	Yellow
LEU	Yellow
ASN	Yellow
LEU	Yellow
LYS	Yellow
ASP	Yellow
LEU	Yellow
LYS	Yellow
ASN	Yellow
ILE	Yellow
PRO	Yellow
GLY	Yellow
ILE	Yellow
GLY	Yellow
GLU	Yellow
ARG	Yellow
SER	Yellow
LEU	Yellow
GLU	Yellow
GLU	Yellow
ILE	Yellow
LYS	Yellow
GLU	Yellow
ALA	Yellow
LEU	Yellow
GLU	Yellow
LYS	Yellow
GLY	Yellow
PHR	Yellow
THR	Yellow
LEU	Yellow
LYS	Yellow
GLU	Yellow

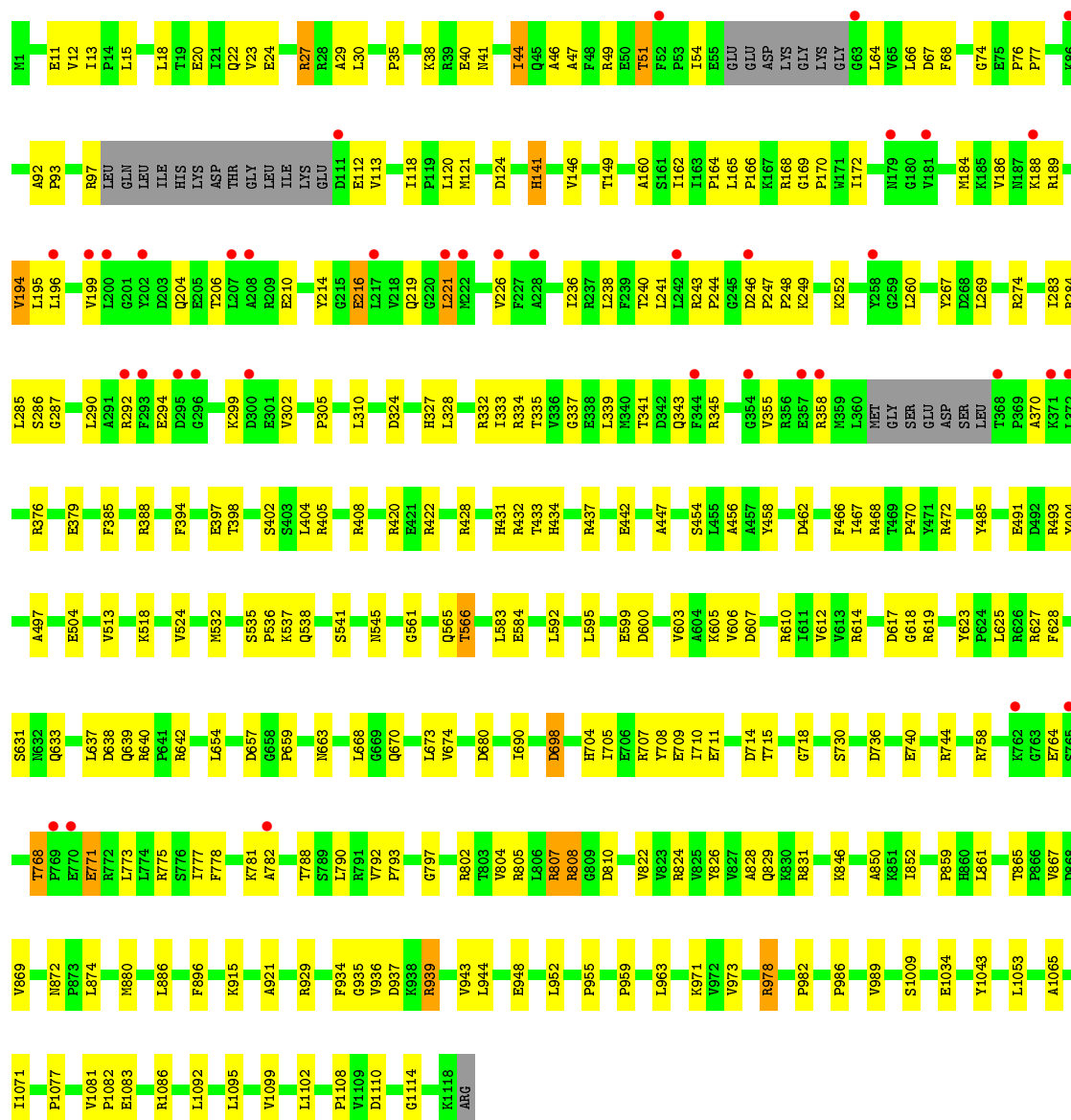
56% 14% 30%

Residue	Category
MET	Grey
LEU	Grey
ASP	Grey
SER	Grey
LYS	Green
LEU	Green
VAL	Yellow
T15	Yellow
R30	Yellow
P39	Yellow
S47	Yellow
T48	Yellow
P49	Yellow
A52	Yellow
Y57	Yellow
L80	Yellow
R83	Yellow
E84	Yellow
L85	Yellow
V86	Yellow
V87	Yellow
L90	Yellow
ASN	Grey
P92	Yellow
L100	Yellow
P106	Yellow
R107	Yellow
E108	Yellow
V109	Yellow
K110	Yellow
R111	Yellow
R112	Yellow
L115	Yellow
P116	Yellow
P125	Yellow
D126	Yellow
L127	Green
H128	Yellow
T131	Yellow
L132	Yellow
L138	Yellow
E144	Yellow

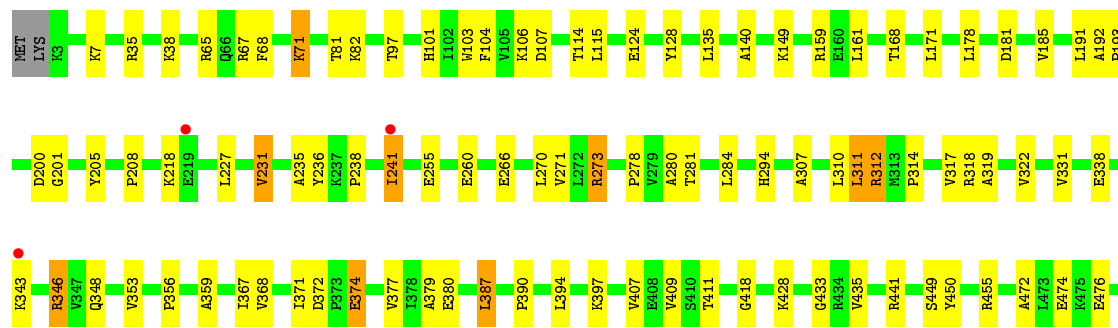
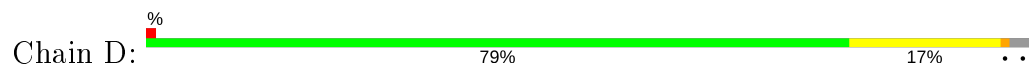
Residue	Category
Y150	Yellow
E154	Yellow
R161	Yellow
T162	Green
M163	Yellow
D168	Yellow
A169	Green
V170	Yellow
R176	Yellow
T184	Yellow
L197	Yellow
W200	Yellow
Q213	Yellow
E216	Yellow
I217	Yellow
L218	Yellow
R219	Yellow
L222	Yellow
P228	Yellow
GLN	Grey
ALA	Grey
ALA	Grey
VAL	Grey
ALA	Grey
ALA	Grey
PRO	Grey
GLU	Grey
GLU	Grey
ALA	Grey
LYS	Grey
GLU	Grey
PRO	Grey
GLU	Grey
GLN	Grey
GLU	Grey
LEU	Grey
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GLU	Grey
LEU	Grey
GLU	Grey
GLU	Grey
GLU	Grey

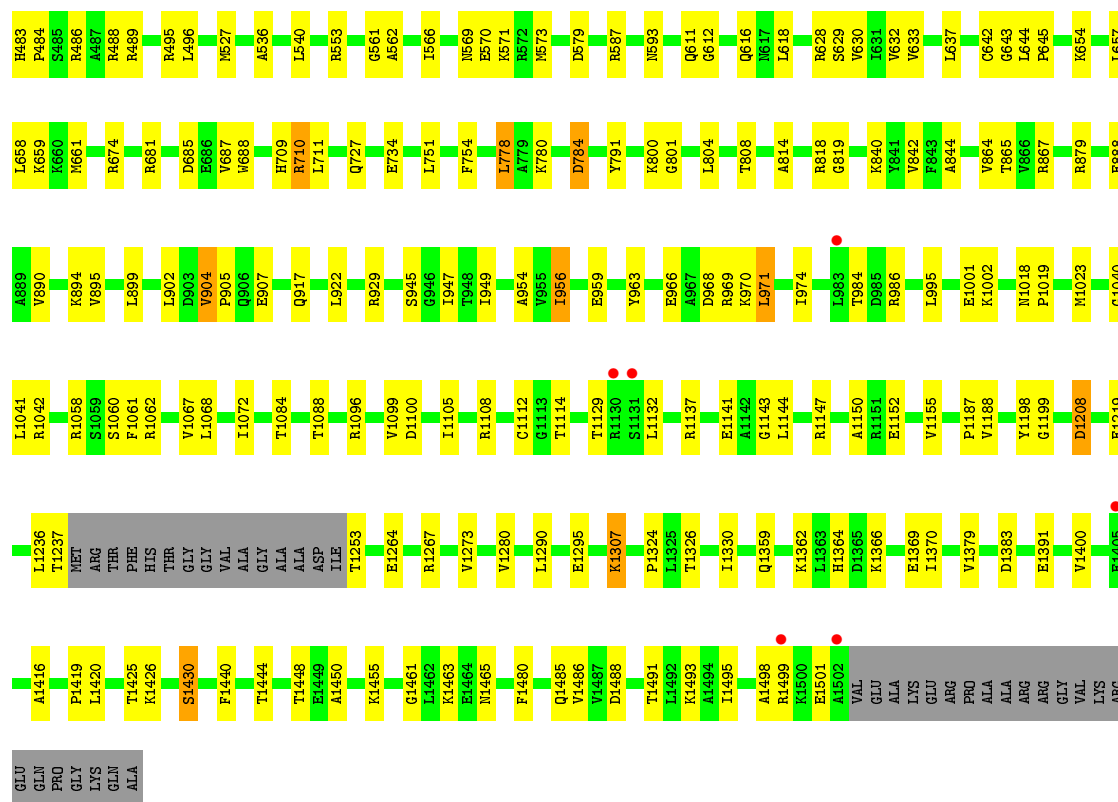
[illegible]



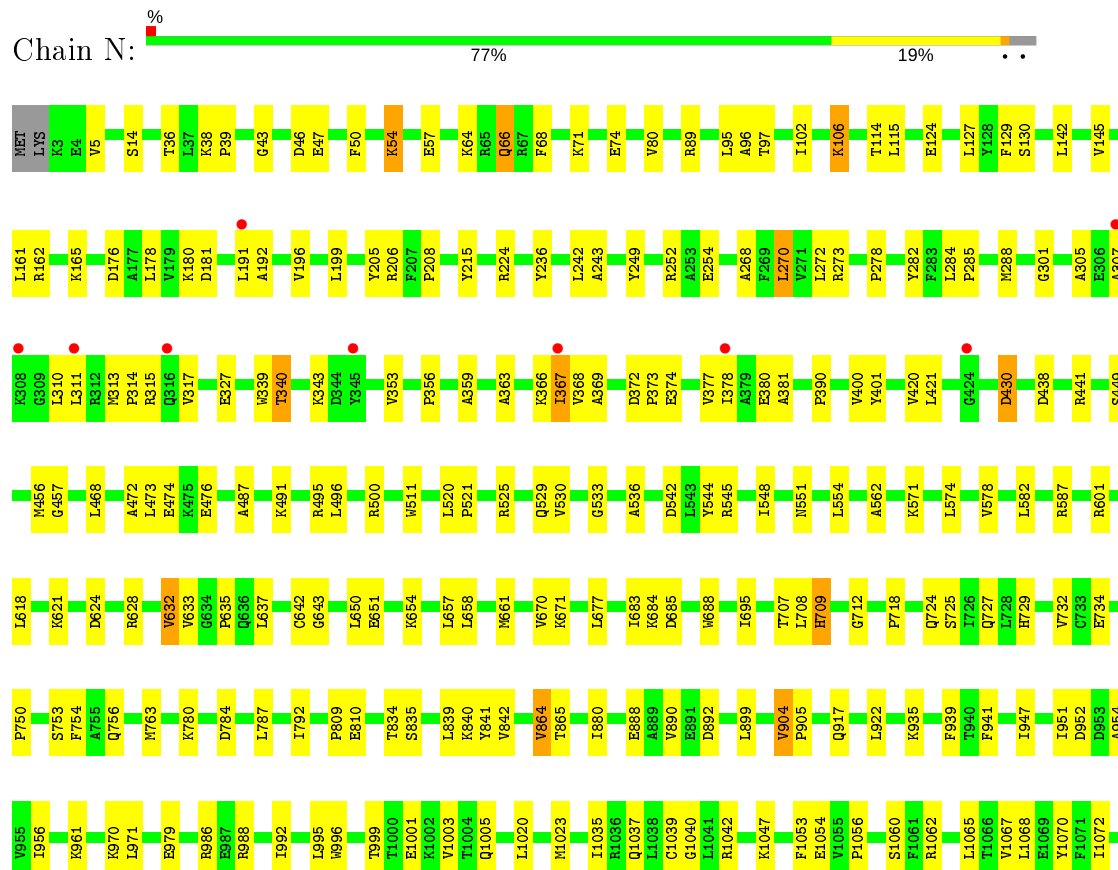


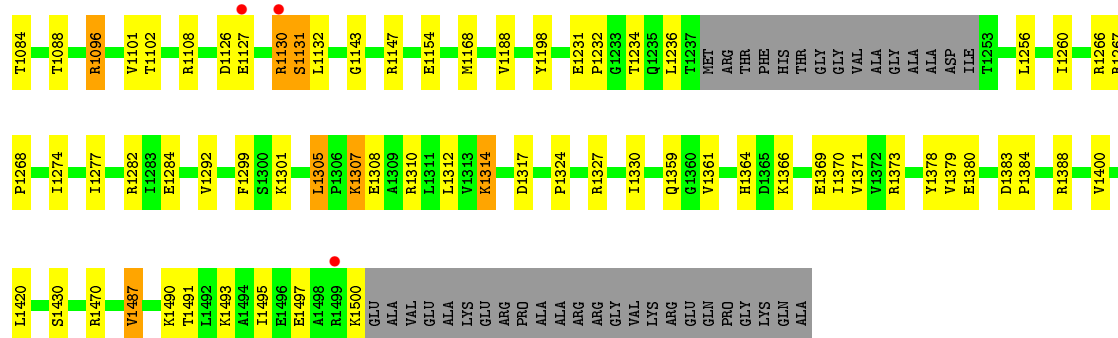
• Molecule 3: DNA-directed RNA polymerase subunit beta'



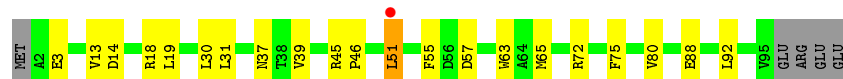


• Molecule 3: DNA-directed RNA polymerase subunit beta'

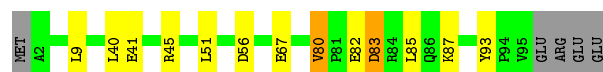
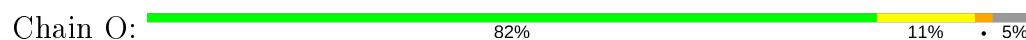




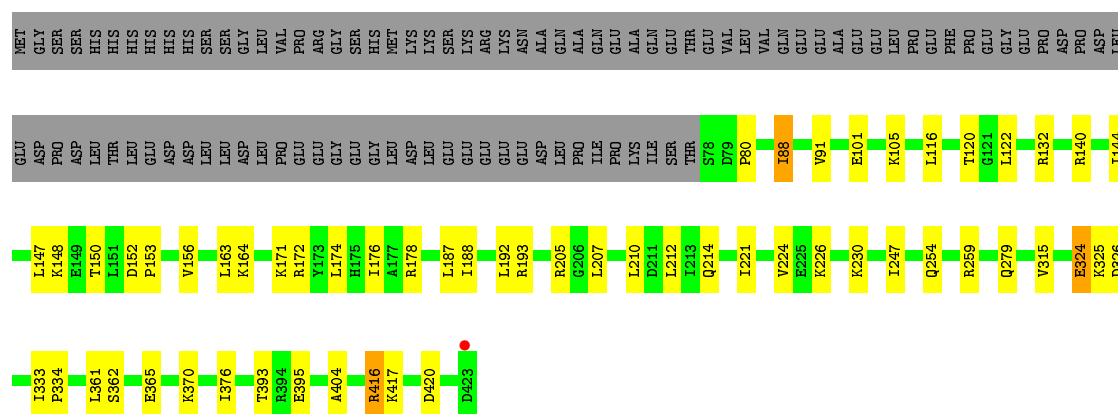
• Molecule 4: DNA-directed RNA polymerase subunit omega



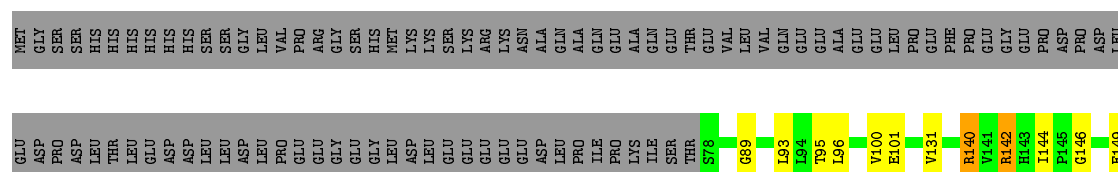
• Molecule 4: DNA-directed RNA polymerase subunit omega

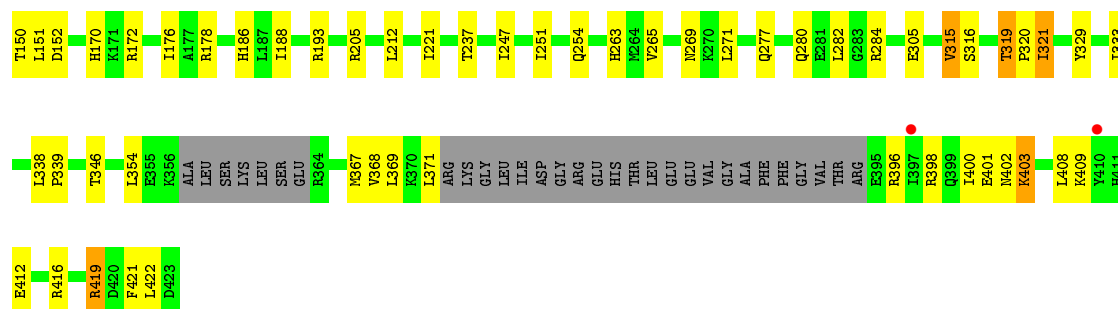


• Molecule 5: RNA polymerase sigma factor SigA



• 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 1.8-1069	Depositor
R, $R_{free}$	0.201 , 0.254 0.203 , 0.254	Depositor DCC
$R_{free}$ test set	10942 reflections (5.00%)	wwPDB-VP
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 [i](#)

### 5.1 Standard geometry [i](#)

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
3:N:643:GLY:HA3	3:N:727:GLN:HB2	1.84	0.59
2:M:872:ASN:ND2	3:N:784:ASP:OD2	2.35	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:1364:HIS:ND1	3:N:1366:LYS:HG2	2.18	0.59
3:N:954:ALA:O	3:N:1062:ARG:NH2	2.35	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:787:LEU:HD21	3:N:947:ILE:HG21	1.88	0.56
3:N:89:ARG:NH1	14:N:2103:HOH:O	2.33	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
2:C:405:ARG:HD3	2:C:566:THR:HG21	1.88	0.55
1:A:70:GLY:N	2:C:607:ASP:OD1	2.37	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:996:TRP:CD2	3:N:1056:PRO:HG3	2.43	0.54
3:N:236:TYR:HB3	3:N:313:MET:HG3	1.90	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
3:D:1426:LYS:O	3:D:1430:SER:OG	2.21	0.53
2:C:872:ASN:ND2	3:D:784:ASP:OD1	2.40	0.53
3:N:529:GLN:NE2	3:N:533:GLY:O	2.41	0.53
3:N:999:THR:O	3:N:1003:VAL:HG23	2.09	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
2:M:915:LYS:NZ	3:N:952:ASP:OD2	2.44	0.51
3:N:181:ASP:HB2	3:N:205:TYR:CD1	2.46	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:L:57:TYR:CE1	1:L:163:ASN:HB2	2.46	0.51
1:K:36:LEU:HD11	1:L:221:HIS:HB3	1.93	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
1:L:80:LEU:HD21	3:N:842:VAL:HG12	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: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:536:PRO:HB3	3:N:1067:VAL:HG21	1.94	0.49
2:M:603:VAL:HG11	2:M:606:VAL:HG23	1.95	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:152:ASP:N	5:P:152:ASP:OD1	2.45	0.49
5:P:131:VAL:HG13	5:P:178:ARG:HD3	1.94	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:227:LEU:HD13	3:D:331:VAL:HB	1.95	0.48
3:D:208:PRO:HG2	3:D:353:VAL:HG21	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:595:LEU:HB3	2:C:656:ALA:HB3	1.98	0.46
2:C:63:GLY:HA3	2:C:100:LEU:HD11	1.96	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:1480:PHE:O	4:E:18:ARG:NH2	2.50	0.45
3:D:409:VAL:HG13	3:D:435:VAL:HG11	1.97	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:243:ALA:HB3	3:N:311:LEU:HD12	1.99	0.45
3:N:162:ARG:O	3:N:449:SER:HB2	2.17	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:243:ARG:HH12	7:S:9:DG:H1	1.64	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
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: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
1:K:83:LYS:NZ	2:M:698:ASP:OD1	2.51	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:1031:ARG:HG2	6:G:16:DT:H5"	2.01	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
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:966:GLU:O	3:D:969:ARG:HB3	2.18	0.43
3:D:573:MET:SD	5:F:210:LEU:HB3	2.58	0.43
2:M:1043:TYR:CG	3:N:763:MET:HG2	2.54	0.43
3:N:127:LEU:HA	3:N:457:GLY:HA2	2.00	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:97:THR:HG21	3:D:571:LYS:HG2	2.02	0.41
3:D:879:ARG:HD3	3:D:902:LEU:O	2.21	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:141:HIS:CE1	2:M:334:ARG:HD2	2.56	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
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:20:TYR:OH	1:K:198:ARG:HD2	2.20	0.41
1:K:41:ARG:HA	1:K:177:VAL:HG11	2.03	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:9:PRO:HB3	1:A:27:PRO:O	2.20	0.41
1:A:218:LEU:HG	1:B:222:LEU:HD11	2.03	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
1:K:70:GLY:H	2:M:607:ASP:CG	2.23	0.40
2:M:274:ARG:HH12	2:M:286:SER:C	2.24	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%)	51	85
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%)	36	71
1	B	195/273 (71%)	189 (97%)	6 (3%)	40	75
1	K	199/273 (73%)	193 (97%)	6 (3%)	41	75
1	L	195/273 (71%)	189 (97%)	6 (3%)	40	75
2	C	933/941 (99%)	899 (96%)	34 (4%)	35	70
2	M	917/941 (97%)	876 (96%)	41 (4%)	27	64
3	D	1252/1279 (98%)	1196 (96%)	56 (4%)	27	64
3	N	1251/1279 (98%)	1195 (96%)	56 (4%)	27	64
4	E	82/88 (93%)	79 (96%)	3 (4%)	34	70
4	O	82/88 (93%)	77 (94%)	5 (6%)	18	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	F	301/388 (78%)	293 (97%)	8 (3%)	44	77
5	P	277/388 (71%)	258 (93%)	19 (7%)	15	48
All	All	5883/6484 (91%)	5636 (96%)	247 (4%)	30	66

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
11	CTP	D	2006	8	6,8,30	1.70	1 (16%)	13,13,47	1.42	1 (7%)
11	CTP	M	1201	8	6,8,30	1.07	1 (16%)	13,13,47	1.23	1 (7%)
12	NAD	D	2008	10	42,48,48	2.16	11 (26%)	50,73,73	1.30	6 (12%)

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
11	CTP	D	2006	8	-	0/6/6/38	-
11	CTP	M	1201	8	-	0/6/6/38	-
12	NAD	D	2008	10	-	9/26/62/62	0/5/5/5

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	2008	NAD	C7N-N7N	5.92	1.44	1.33
12	D	2008	NAD	O4B-C1B	5.67	1.49	1.41
12	D	2008	NAD	O4D-C1D	5.33	1.48	1.41
12	D	2008	NAD	C2A-N3A	4.65	1.39	1.32
11	D	2006	CTP	PA-O1A	3.74	1.62	1.50
12	D	2008	NAD	C2A-N1A	3.38	1.40	1.33
12	D	2008	NAD	O2D-C2D	-2.85	1.36	1.43
12	D	2008	NAD	C6A-N6A	2.61	1.43	1.34
12	D	2008	NAD	O2B-C2B	-2.51	1.37	1.43
12	D	2008	NAD	C6A-C5A	-2.26	1.34	1.43
12	D	2008	NAD	O3D-C3D	-2.18	1.37	1.43
12	D	2008	NAD	C2B-C3B	-2.11	1.47	1.53
11	M	1201	CTP	PA-O5'	2.07	1.62	1.54

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	D	2008	NAD	N3A-C2A-N1A	-4.61	121.47	128.68
11	D	2006	CTP	PB-O3A-PA	-3.76	119.92	132.83
12	D	2008	NAD	PN-O3-PA	-3.75	119.96	132.83
11	M	1201	CTP	PB-O3A-PA	-3.14	122.04	132.83
12	D	2008	NAD	C3N-C7N-N7N	3.12	121.49	117.75
12	D	2008	NAD	O7N-C7N-N7N	-2.51	119.02	122.58
12	D	2008	NAD	C2D-C3D-C4D	2.50	107.50	102.64
12	D	2008	NAD	C4A-C5A-N7A	2.39	111.89	109.40

There are no chirality outliers.

All (9) torsion outliers are listed below:

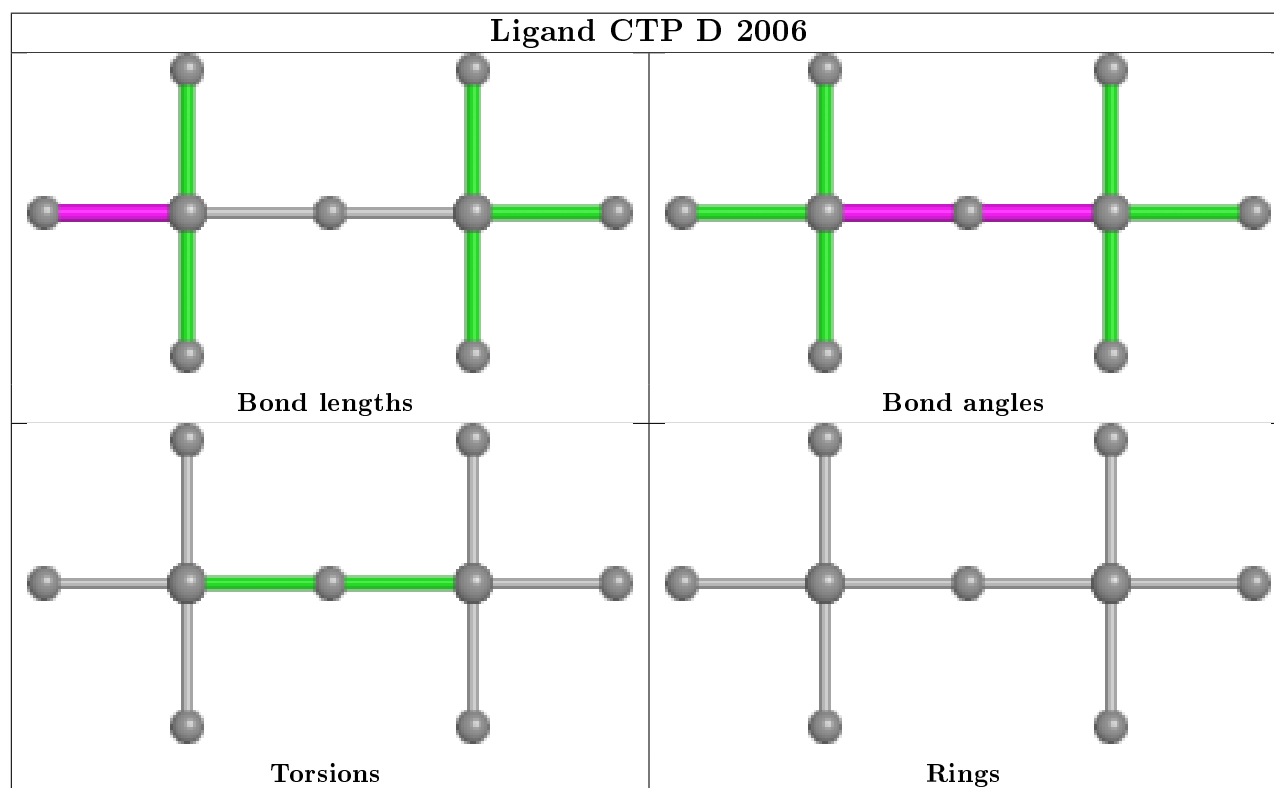
Mol	Chain	Res	Type	Atoms
12	D	2008	NAD	C5B-O5B-PA-O3
12	D	2008	NAD	PN-O3-PA-O5B
12	D	2008	NAD	O4B-C4B-C5B-O5B
12	D	2008	NAD	C5D-O5D-PN-O3
12	D	2008	NAD	C5D-O5D-PN-O2N
12	D	2008	NAD	C3B-C4B-C5B-O5B
12	D	2008	NAD	C5B-O5B-PA-O2A
12	D	2008	NAD	C5D-O5D-PN-O1N
12	D	2008	NAD	PN-O3-PA-O1A

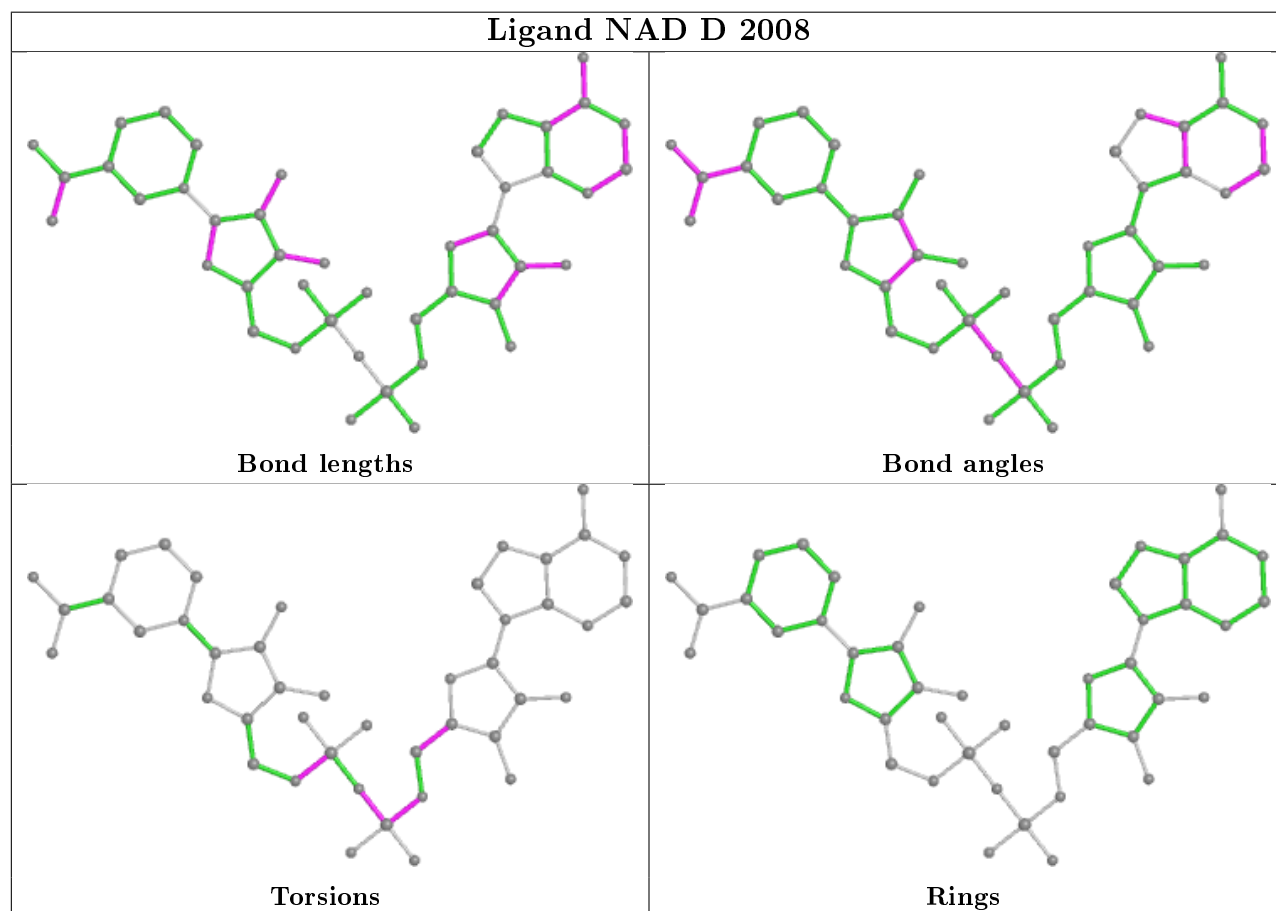
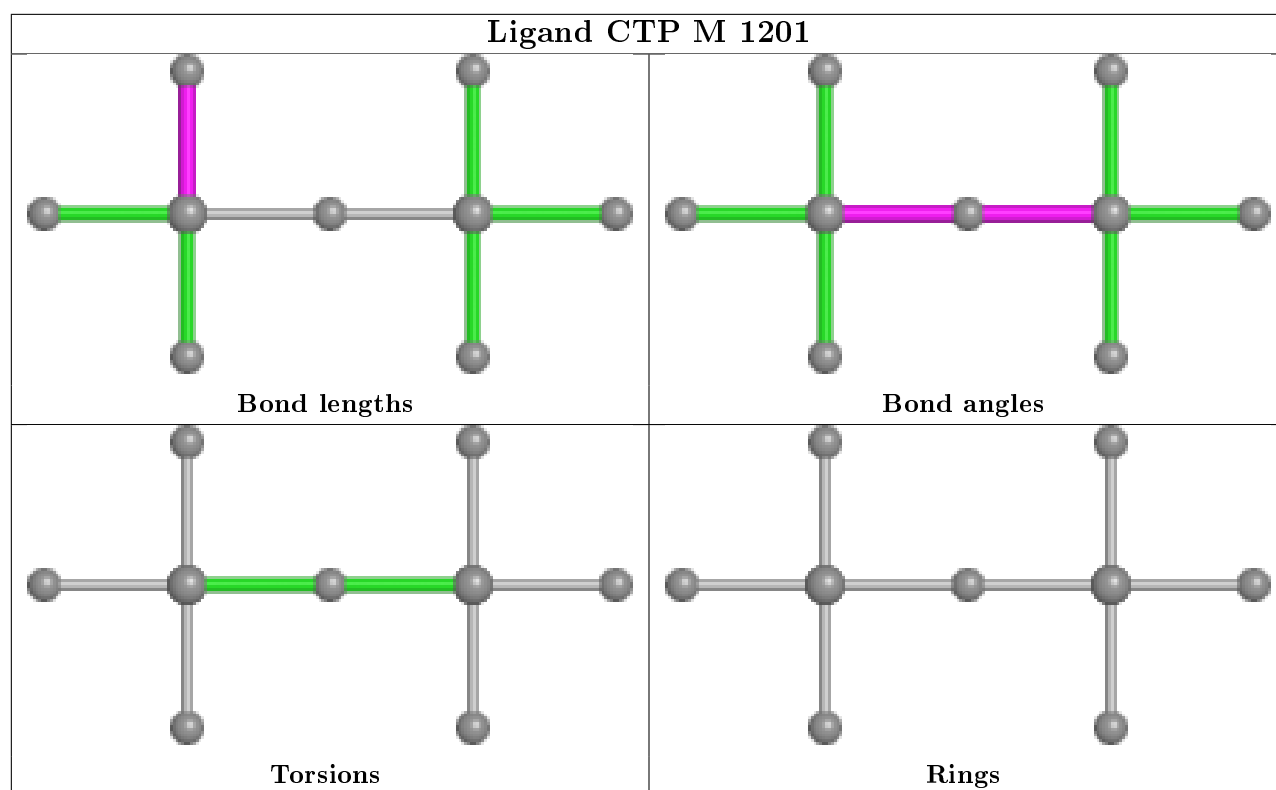
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	D	2008	NAD	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 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%) 92 79	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%)	-0.45	5 (0%) 91 75	0, 14, 62, 89	3 (0%)
2	M	1091/1119 (97%)	-0.12	38 (3%) 44 18	1, 39, 97, 116	2 (0%)
3	D	1485/1524 (97%)	-0.36	9 (0%) 89 72	0, 18, 68, 103	4 (0%)
3	N	1483/1524 (97%)	-0.30	12 (0%) 86 65	0, 24, 77, 106	4 (0%)
4	E	94/99 (94%)	-0.55	1 (1%) 80 56	1, 13, 49, 67	0
4	O	94/99 (94%)	-0.40	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	2 (0%) 89 72	17, 46, 91, 109	0
6	G	16/19 (84%)	-0.14	1 (6%) 20 6	16, 48, 112, 117	0
6	R	16/19 (84%)	-0.08	0 100 100	39, 65, 115, 122	0
7	H	21/27 (77%)	-0.18	1 (4%) 30 11	19, 56, 108, 124	0
7	S	21/27 (77%)	0.04	1 (4%) 30 11	33, 84, 121, 144	0
All	All	6992/7722 (90%)	-0.33	72 (1%) 82 59	0, 26, 78, 144	15 (0%)

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	188	LYS	5.0
2	M	200	LEU	4.4
2	M	196	LEU	4.4
2	M	63	GLY	3.8
2	M	368	THR	3.7

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Mol	Chain	Res	Type	RSRZ
2	M	765	SER	3.6
2	M	217	LEU	3.5
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
3	D	1130	ARG	2.9
2	M	358	ARG	2.9
3	N	191	LEU	2.8
2	M	258	TYR	2.8
5	P	410	TYR	2.7
2	M	762	LYS	2.7
3	D	1499	ARG	2.6
2	M	181	VAL	2.6
2	M	295	ASP	2.6
2	M	52	PHE	2.6
4	E	51	LEU	2.6
3	D	241	ILE	2.5
2	M	371	LYS	2.5
2	C	104	ASP	2.5
3	N	1130	ARG	2.5
2	M	179	ASN	2.5
2	C	205	GLU	2.5
2	M	769	PRO	2.4
2	M	226	VAL	2.4
2	M	782	ALA	2.4
2	C	105	THR	2.4
3	N	345	TYR	2.4
3	N	367	ILE	2.4
1	A	231	ALA	2.4
3	N	424	GLY	2.3
3	N	378	ILE	2.3
2	M	296	GLY	2.3
7	H	25	DA	2.3
3	N	311	LEU	2.3
3	N	307	ALA	2.3
3	N	316	GLN	2.3
2	M	242	LEU	2.2
5	F	423	ASP	2.2
2	M	246	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
3	N	1499	ARG	2.2
2	M	208	ALA	2.2
3	D	219	GLU	2.2
2	M	354	GLY	2.2
3	D	1405	GLU	2.2
5	P	397	ILE	2.1
3	N	1127	GLU	2.1
2	M	86	LYS	2.1
2	M	111	ASP	2.1
3	D	1131	SER	2.1
3	D	1502	ALA	2.1
7	S	25	DA	2.1
3	D	343	LYS	2.1
3	N	308	LYS	2.1
2	M	372	LEU	2.1
2	M	222	MET	2.1
2	M	770	GLU	2.1
3	D	983	LEU	2.1
2	M	344	PHE	2.0
2	M	357	GLU	2.0
6	G	4	DT	2.0
2	M	292	ARG	2.0
2	M	293	PHE	2.0
2	M	221	LEU	2.0
2	M	300	ASP	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

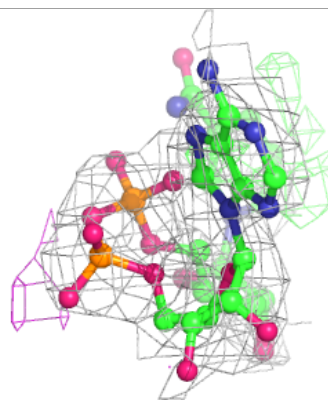
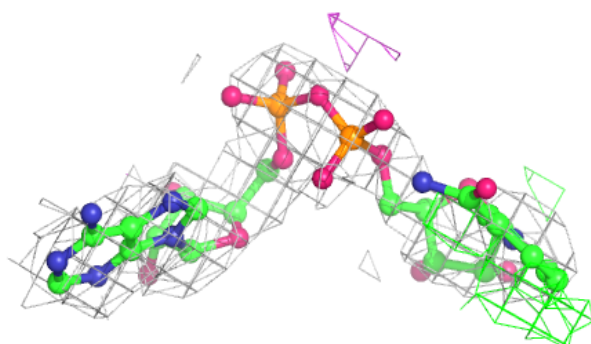
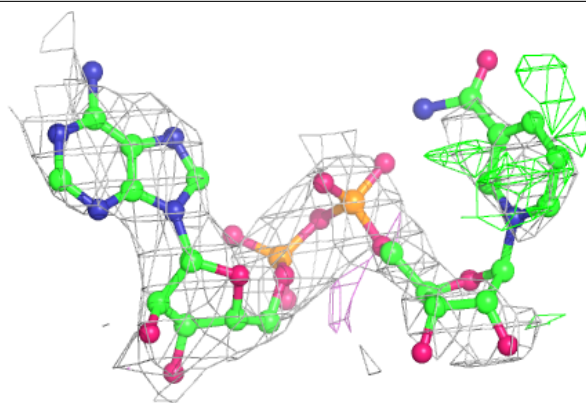


Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
13	A	R	101	23/23	0.82	0.26	37,54,63,83	23
8	MG	D	2003	1/1	0.88	0.23	1,1,1,1	0
10	C	N	2005	20/21	0.88	0.23	22,46,53,59	20
12	NAD	D	2008	44/44	0.89	0.24	15,34,53,67	44
11	CTP	M	1201	9/29	0.89	0.20	25,52,69,73	0
11	CTP	D	2006	9/29	0.91	0.20	21,41,62,80	0
8	MG	P	2001	1/1	0.91	0.24	51,51,51,51	0
8	MG	B	2001	1/1	0.92	0.20	17,17,17,17	0
8	MG	N	2003	1/1	0.93	0.26	6,6,6,6	0
8	MG	F	2001	1/1	0.93	0.06	25,25,25,25	0
8	MG	L	2001	1/1	0.93	0.10	41,41,41,41	0
10	C	D	2005	20/21	0.94	0.18	6,19,38,47	20
8	MG	N	2006	1/1	0.94	0.28	32,32,32,32	0
8	MG	D	2007	1/1	0.94	0.33	28,28,28,28	0
9	ZN	N	2002	1/1	0.96	0.07	89,89,89,89	0
8	MG	N	2004	1/1	0.98	0.07	27,27,27,27	0
9	ZN	D	2002	1/1	0.99	0.05	40,40,40,40	0
9	ZN	D	2001	1/1	0.99	0.14	5,5,5,5	0
8	MG	D	2004	1/1	0.99	0.18	15,15,15,15	0
9	ZN	N	2001	1/1	1.00	0.15	7,7,7,7	0

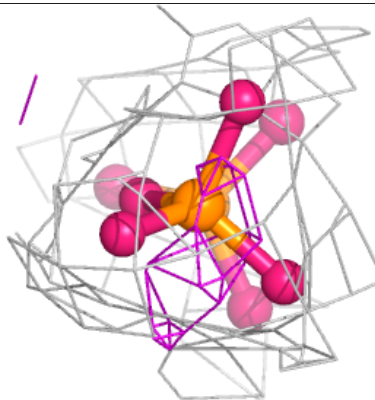
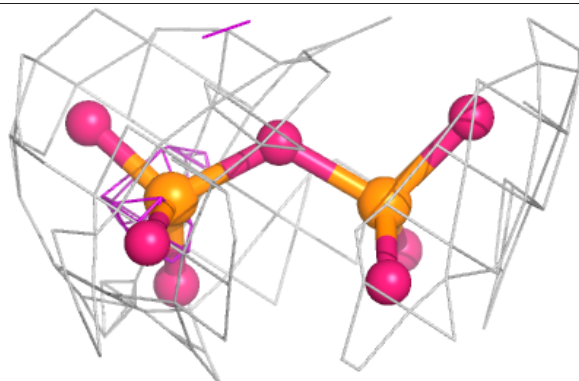
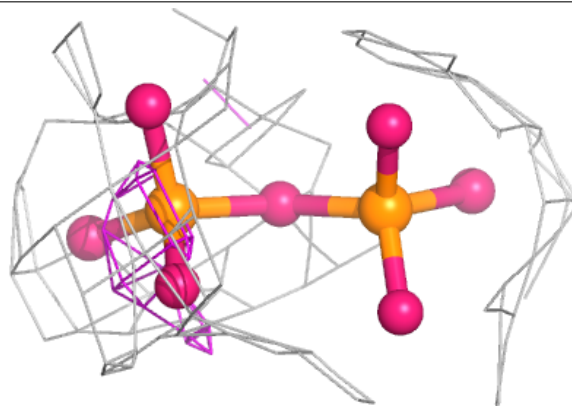
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around NAD D 2008:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

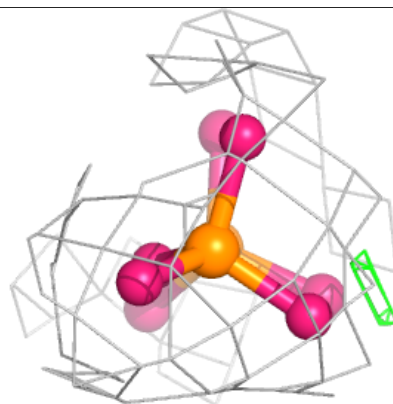
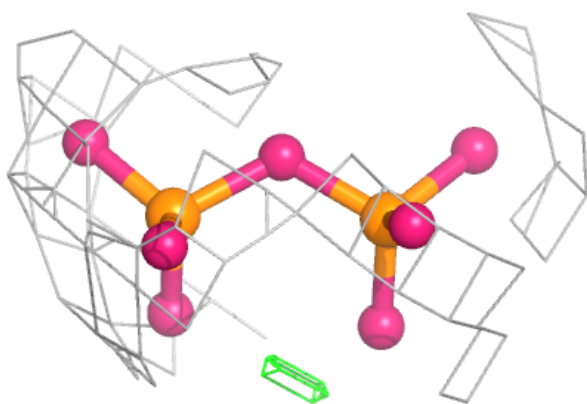
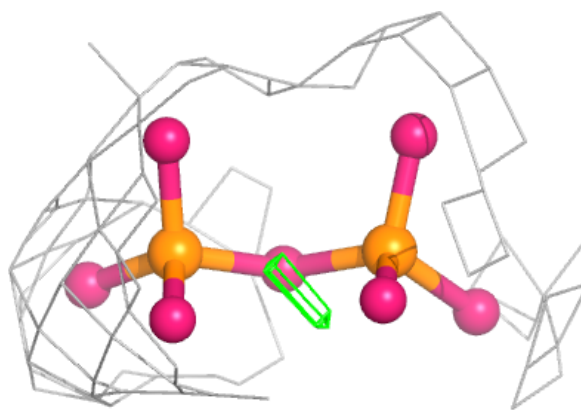
**Electron density around CTP M 1201:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CTP D 2006:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.