



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 11:52 pm BST

PDB ID : 5D4E
Title : Crystal structure of Thermus thermophilus product complex for transcription initiation with 3'-dephosphate-CoA and CTP
Authors : Zhang, Y.; Ebright, R.H.
Deposited on : 2015-08-07
Resolution : 3.08 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (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

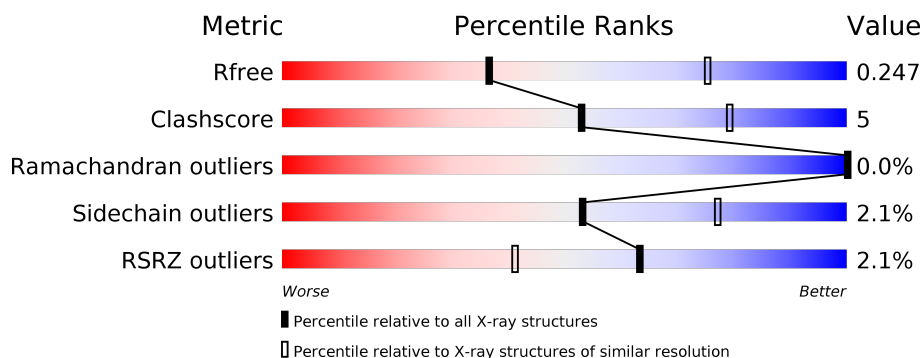
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.08 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	1447 (3.10-3.06)
Clashscore	141614	1546 (3.10-3.06)
Ramachandran outliers	138981	1487 (3.10-3.06)
Sidechain outliers	138945	1486 (3.10-3.06)
RSRZ outliers	127900	1416 (3.10-3.06)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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>2%</div> <div> <div></div> <div>61%</div> <div>12%</div> <div>•</div> <div>27%</div> </div> </div>
1	B	315	<div> <div>%</div> <div> <div></div> <div>61%</div> <div>10%</div> <div></div> <div>29%</div> </div> </div>
1	K	315	<div> <div>2%</div> <div> <div></div> <div>61%</div> <div>12%</div> <div></div> <div>27%</div> </div> </div>
1	L	315	<div> <div></div> <div> <div></div> <div>60%</div> <div>11%</div> <div></div> <div>29%</div> </div> </div>
2	C	1119	<div> <div>4%</div> <div> <div></div> <div>81%</div> <div>18%</div> <div>••</div> </div> </div>
2	M	1119	<div> <div>%</div> <div> <div></div> <div>85%</div> <div>14%</div> <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	H	27	
6	S	27	
7	G	19	
7	R	19	

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
12	COD	D	2008	-	-	-	X

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 57723 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	231	Total	C	N	O	S	0	0	0
			1809	1155	315	337	2			
1	B	223	Total	C	N	O	S	0	0	0
			1758	1124	305	327	2			
1	K	231	Total	C	N	O	S	0	0	0
			1809	1155	315	337	2			
1	L	223	Total	C	N	O	S	0	0	0
			1758	1124	305	327	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1112	Total	C	N	O	S	0	0	0
			8774	5550	1565	1635	24			
2	M	1112	Total	C	N	O	S	0	1	0
			8783	5558	1565	1636	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1486	Total	C	N	O	S	0	0	0
			11738	7441	2067	2195	35			
3	N	1486	Total	C	N	O	S	0	0	0
			11738	7441	2067	2195	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	346	Total	C	N	O	S	0	0	0
			2807	1770	509	524	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 (27-MER).

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

- Molecule 7 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
7	G	16	Total	C	N	O	P	0	0	0
			327	156	62	94	15			
7	R	16	Total	C	N	O	P	0	0	0
			328	157	62	94	15			

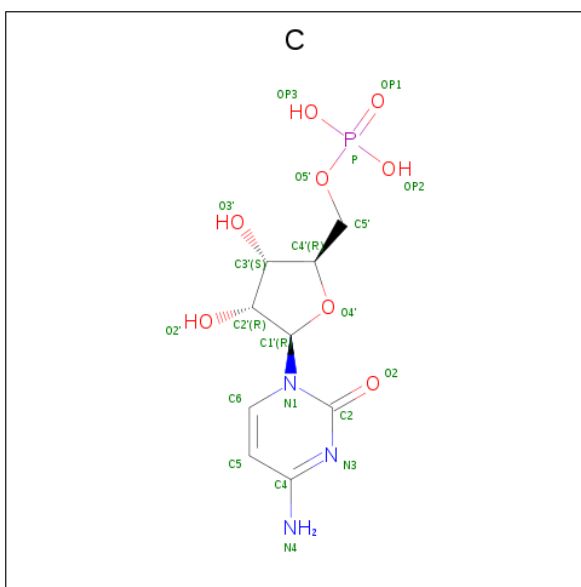
- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

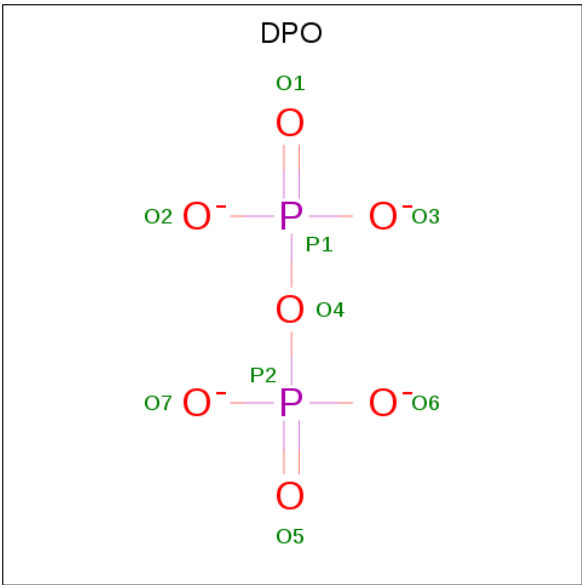
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	D	2	Total	Zn	0	0
			2	2		
9	N	2	Total	Zn	0	0
			2	2		

- Molecule 10 is CYTIDINE-5'-MONOPHOSPHATE (three-letter code: C) (formula: $C_9H_{14}N_3O_8P$).



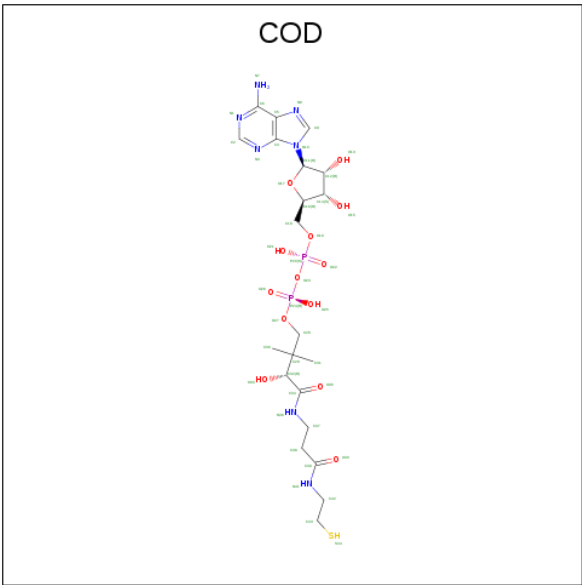
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	D	1	Total	C	N	O	P	0	0
			20	9	3	7	1		
10	N	1	Total	C	N	O	P	0	0
			20	9	3	7	1		

- Molecule 11 is DIPHOSPHATE (three-letter code: DPO) (formula: O_7P_2).



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

- Molecule 12 is DEPHOSPHO COENZYME A (three-letter code: COD) (formula: C₂₁H₃₅N₇O₁₃P₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	D	1	Total	C	N	O	P	0	0
			28	11	5	10	2		
12	N	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

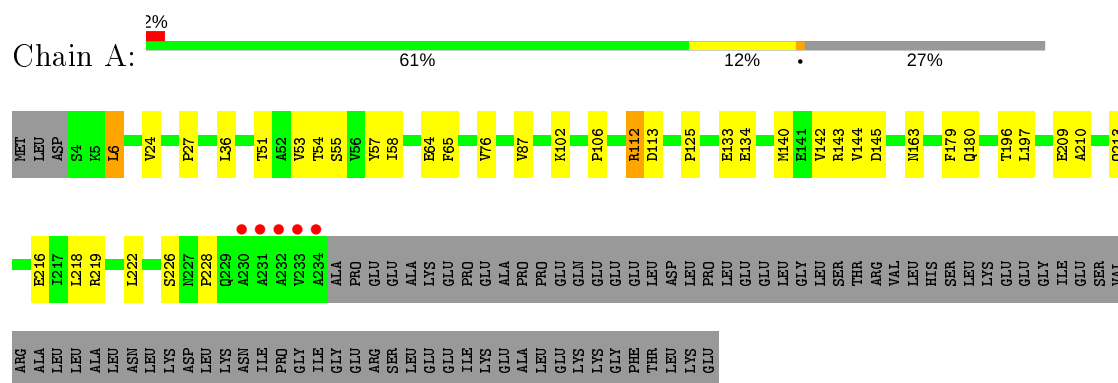
- Molecule 13 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	17	Total O 17 17	0	0
13	B	10	Total O 10 10	0	0
13	C	74	Total O 74 74	0	0
13	D	144	Total O 144 144	0	0
13	E	8	Total O 8 8	0	0
13	F	17	Total O 17 17	0	0
13	H	6	Total O 6 6	0	0
13	G	3	Total O 3 3	0	0
13	K	16	Total O 16 16	0	0
13	L	14	Total O 14 14	0	0
13	M	178	Total O 178 178	0	0
13	N	217	Total O 217 217	0	0
13	O	16	Total O 16 16	0	0
13	P	41	Total O 41 41	0	0
13	R	9	Total O 9 9	0	0
13	S	5	Total O 5 5	0	0

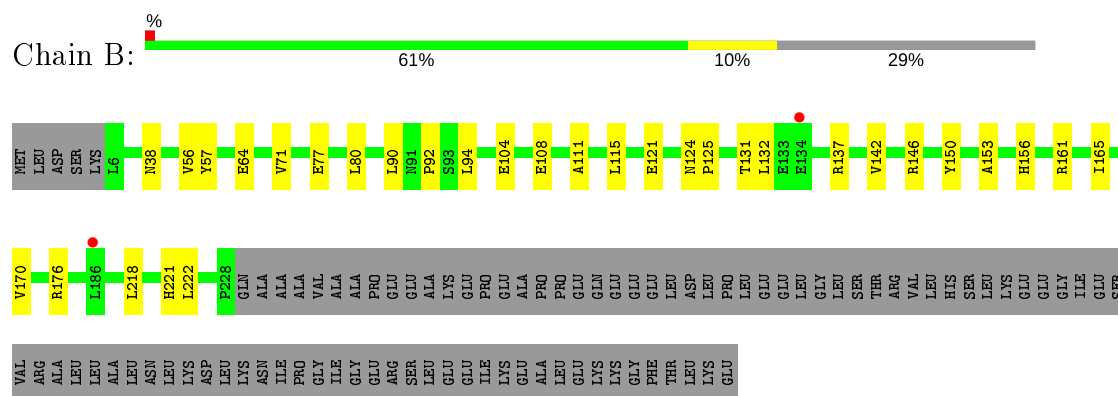
3 Residue-property plots [i](#)

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

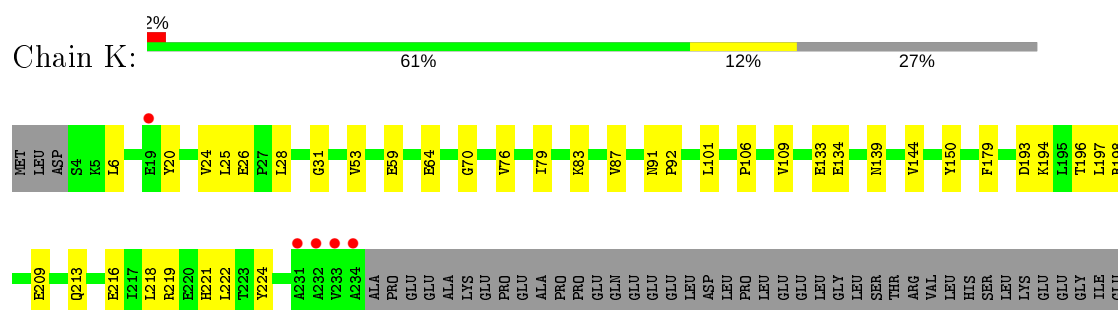
- Molecule 1: DNA-directed RNA polymerase subunit alpha



- Molecule 1: DNA-directed RNA polymerase subunit alpha



- Molecule 1: DNA-directed RNA polymerase subunit alpha



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

MET LEU
LEU
ASP
SER
LVS
L6
K7
A8
P9
F11
V10
F23
F23
TS1
V56
V56
V71
E77
L80
K83
V87
L90
N91
P92
E104
E108
A111
P125
H128
T131
L132
R137
V142
R143
R146
E154
D168
R176
V215

E216
E217
R219
L222
P228
GLN
ALA
ALA
VAL
ALA
ALA
PRO
GLU
GLU
ALA
LYS
GLU
PRO
GLU
ALA
PRO
PRO
GLU
GLN
GLU
GLU
GLU
N91
P92
ASP
LEU
LEU
PRO
GLU
LEU
GLU
GLU
GLY
SER
THR
ARG
VAL
HIS
SER
LEU
LYS
GLU
GLY
ILE
GLU
SER
VAL
ARG
ALA
LEU

LEU
ALA
ASN
LVS
ASP
LEU
LYS
ASN
ILE
PRO
GLY
ILE
GLY
GLU
GLU
LYS
LYS
PHE
THR
LEU
LYS
GLU

- Molecule 2: DNA-directed RNA polymerase subunit beta

Chain C: 

H1
E2
V12
I13
Q22
V23
E24
R27
R28
A32
D33
V34
P35
P36
R38
E40
N41
V42
A46
A47
F48
F52
E55
E56
GLU
ASP
LVS
GLY
LYS
GLY
G63
L64
V65
L66
D67
F68
Y71
R72
L73
K86
D87
H102
K103
D104
T105
G106
L107
I108
K109

E110
D111
E112
I118
T122
E123
G131
H141
V146
P164
L165
R168
I172
V186
N187
K188
L196
L200
G201
Y202
L207
L221
M222
D223
E224
S225
V226
E232
T240
L241
L242
D246
P247
P248
K249
R250
D251
V254
A255
Y258
I261

R266
Y267
L269
K276
L281
G282
I283
R284
S286
G287
L290
A291
R292
F293
D294
D295
G296
K299
D300
E301
F302
F303
L304
P305
D324
H327
K330
R331
R334
D342
R353
R356
E357
R358
R359
L360
H361
G362
S363
D364
D365
S366
L367
A370


S389
Q390
L391
N399
S402
R405
H406
K407
R408
L413
G414
P415
E421
R428
A447
L451
A456
R460
V461
D462
I467
R468
T469
Y471
R472
Y485
A499
E504
A509
R512
V513
L523
V524
D533
V534
S541
N545
Q567

R573
E584
E585
R586
D590
A597
G598
E599
D600
K605
R610
I611
V612
E622
R627
F628
S631
L637
D638
Q639
R640
F641
R642
V649
D657
G658
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D698
F699
I703
V710
E711
A712
R713
D714
T715

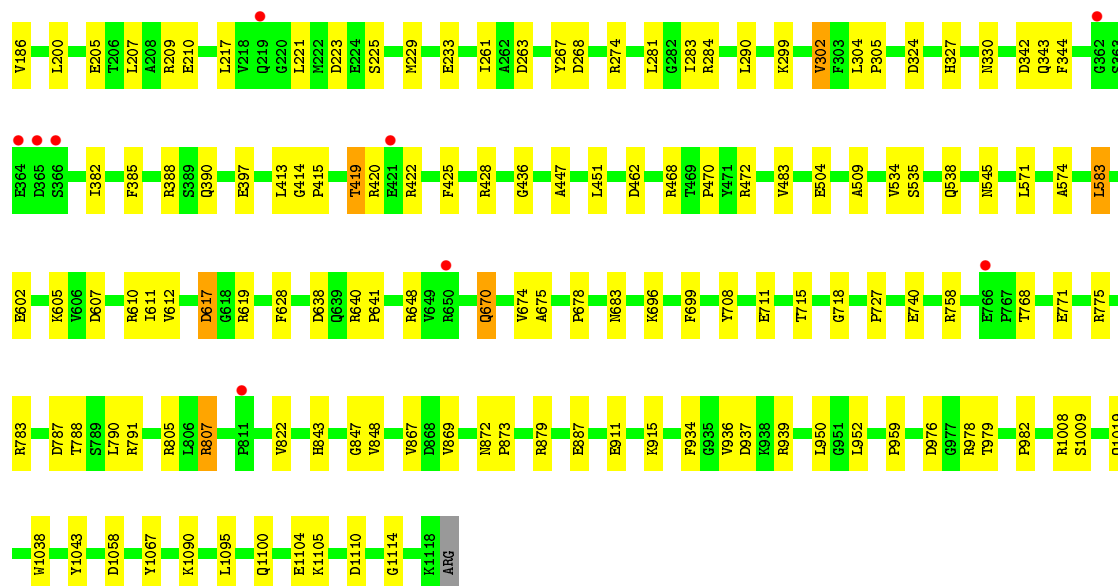
K716
L717
G718
E739
I754
R758
E766
P769
E770
L773
L774
R775
S776
I777
F778
A782
T788
S789
L790
R791
V800
R801
R802
R808
G809
E821
V822
Y826
V827
K838
V869
L874
N881
L886
Q899
R900
Y901
E911
K915

F934
G935
V936
D937
R938
R939
I950
G951
L952
V953
T954
P955
P959
R971
R978
P982
P983
P986
I987
L997
Y998
GLY
S1009
Q1019
W1038
Y1043
E1051
L1055
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D1110
I1111
F1112
E1113
G1114
K1118
ARG

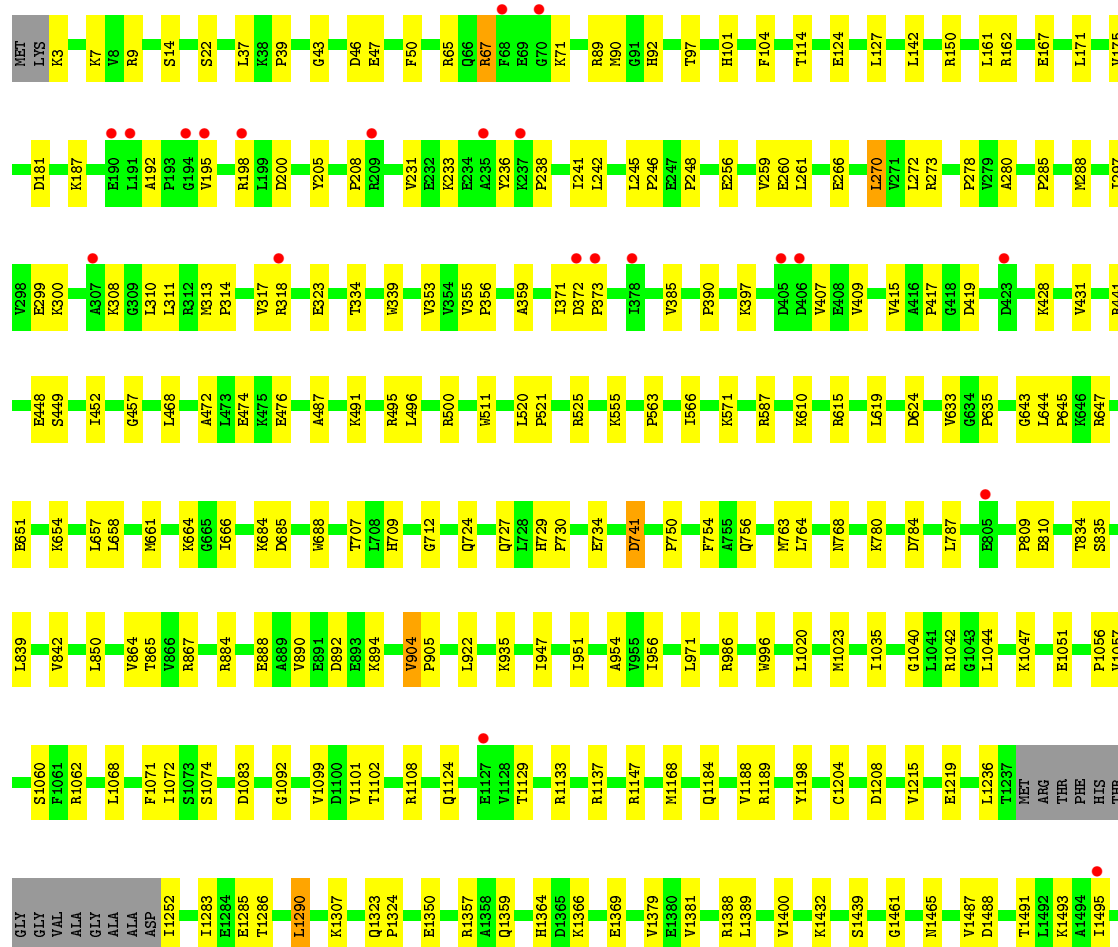
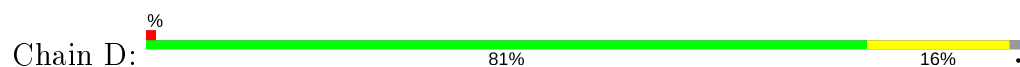
- Molecule 2: DNA-directed RNA polymerase subunit beta

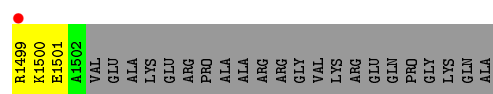
Chain M: 

H1
V12
I13
P17
E20
E24
R27
P35
P36
E40
N41
Q45
A46
E56
GLU
ASP
LYS
LYS
LYS
GLY
G63
E70
A92
H102
K103
D104
I118
P119
L120
D123
H141
A150
L165
R168
I172
D173
L174
E177
P178

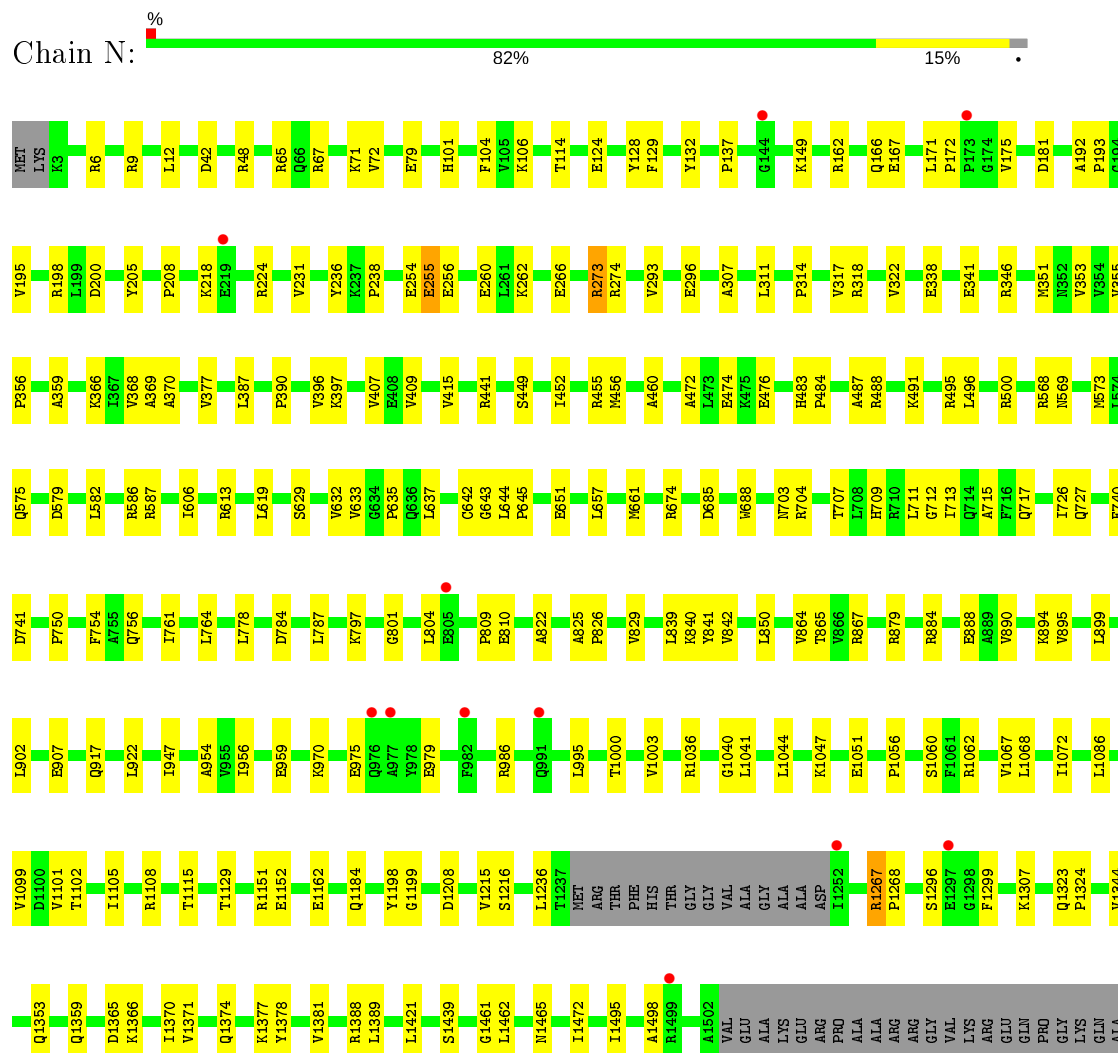


• Molecule 3: DNA-directed RNA polymerase subunit beta'

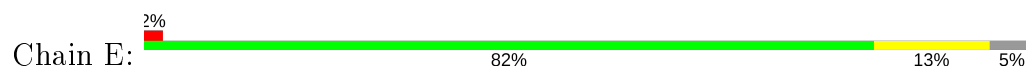




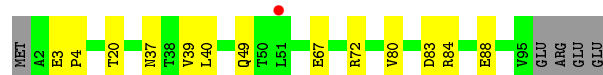
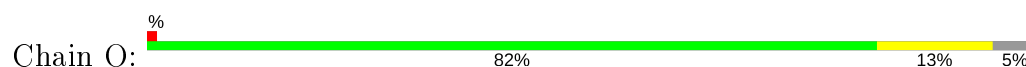
- Molecule 3: DNA-directed RNA polymerase subunit beta'



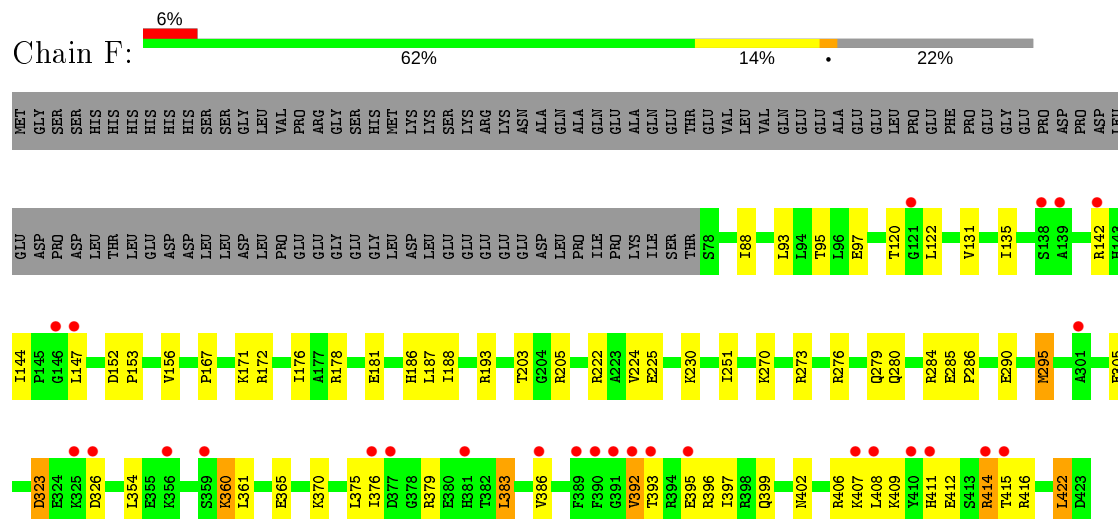
- Molecule 4: DNA-directed RNA polymerase subunit omega



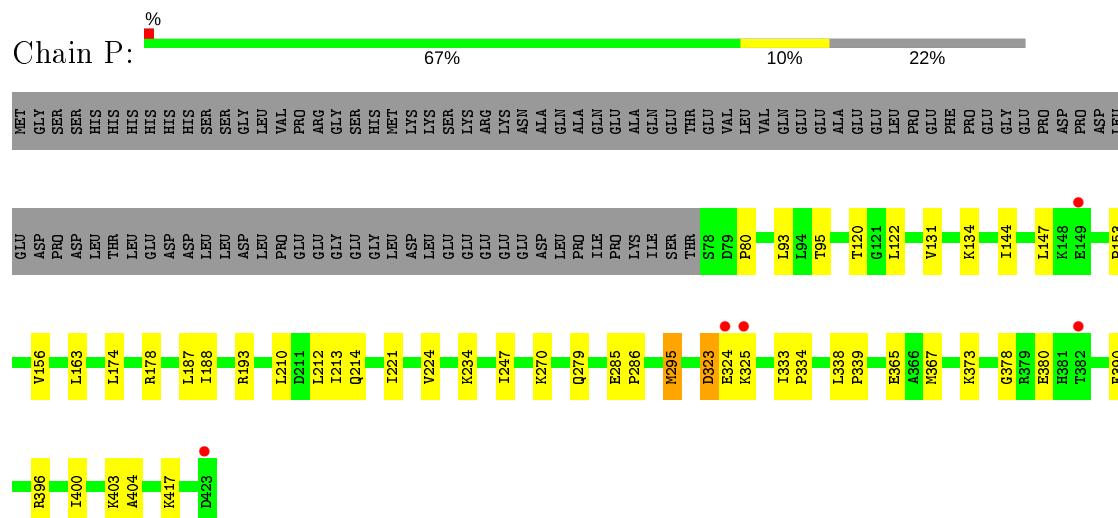
- Molecule 4: DNA-directed RNA polymerase subunit omega



- Molecule 5: RNA polymerase sigma factor SigA



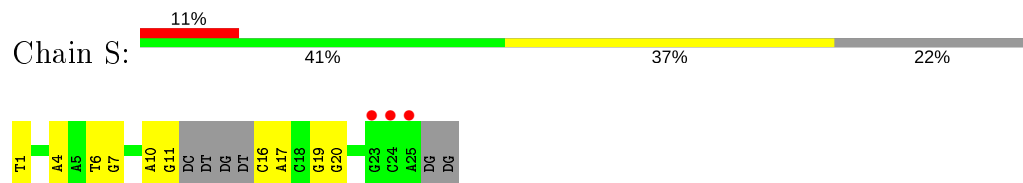
- Molecule 5: RNA polymerase sigma factor SigA



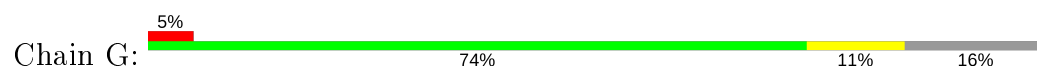
- Molecule 6: DNA (27-MER)



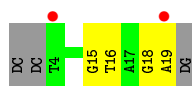
- Molecule 6: DNA (27-MER)



- Molecule 7: 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 (5'-D(*CP*C*TP*GP*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*TP*AP*GP*AP*G)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	185.81Å 103.95Å 297.14Å 90.00° 98.47° 90.00°	Depositor
Resolution (Å)	39.68 – 3.08 39.68 – 3.08	Depositor EDS
% Data completeness (in resolution range)	89.9 (39.68-3.08) 90.0 (39.68-3.08)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 3.06Å)	Xtrriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.210 , 0.246 0.210 , 0.247	Depositor DCC
R_{free} test set	9379 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	62.5	Xtrriage
Anisotropy	0.029	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 38.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	57723	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.93 % 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 1.0674e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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: DPO, MG, ZN, COD

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	0.21	0/1841	0.41	0/2504
1	B	0.26	0/1790	0.45	0/2435
1	K	0.22	0/1841	0.42	0/2504
1	L	0.26	0/1790	0.46	1/2435 (0.0%)
2	C	0.22	0/8941	0.41	0/12092
2	M	0.23	0/8954	0.42	0/12110
3	D	0.21	0/11944	0.40	0/16149
3	N	0.22	0/11944	0.41	0/16149
4	E	0.21	0/772	0.37	0/1040
4	O	0.22	0/772	0.39	0/1040
5	F	0.22	0/2852	0.39	0/3837
5	P	0.21	0/2852	0.38	0/3837
6	H	0.45	0/489	0.99	0/752
6	S	0.45	0/489	1.02	1/752 (0.1%)
7	G	0.44	0/367	0.93	0/565
7	R	0.44	0/368	0.99	1/567 (0.2%)
All	All	0.23	0/58006	0.44	3/78768 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	S	1	DT	O4'-C1'-N1	5.44	111.81	108.00
7	R	16	DT	O4'-C4'-C3'	-5.28	102.39	104.50
1	L	91	ASN	C-N-CD	5.11	139.13	128.40

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	1809	0	1863	24	0
1	B	1758	0	1808	22	0
1	K	1809	0	1863	25	0
1	L	1758	0	1808	21	0
2	C	8774	0	8877	121	0
2	M	8783	0	8886	94	0
3	D	11738	0	11971	136	0
3	N	11738	0	11971	133	0
4	E	758	0	770	6	0
4	O	758	0	770	9	0
5	F	2807	0	2882	42	0
5	P	2807	0	2882	29	0
6	H	435	0	238	4	0
6	S	435	0	238	6	0
7	G	327	0	179	2	0
7	R	328	0	182	2	0
8	B	1	0	0	0	0
8	D	3	0	0	0	0
8	F	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
10	N	20	0	11	2	0
11	D	9	0	0	0	0
11	N	9	0	0	0	0
12	D	28	0	11	0	0
12	N	27	0	11	0	0
13	A	17	0	0	0	0
13	B	10	0	0	0	0
13	C	74	0	0	2	0
13	D	144	0	0	0	0
13	E	8	0	0	0	0
13	F	17	0	0	0	0
13	G	3	0	0	0	0
13	H	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	K	16	0	0	0	0
13	L	14	0	0	0	0
13	M	178	0	0	3	0
13	N	217	0	0	2	0
13	O	16	0	0	0	0
13	P	41	0	0	0	0
13	R	9	0	0	0	0
13	S	5	0	0	0	0
All	All	57723	0	57232	614	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (614) 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:C:628:PHE:H	2:C:638:ASP:HB3	1.40	0.86
2:M:168:ARG:HD3	2:M:268:ASP:HB3	1.64	0.79
2:M:165:LEU:HB2	2:M:168:ARG:HG3	1.63	0.78
2:C:802:ARG:HB2	2:C:826:TYR:HB2	1.66	0.75
2:C:165:LEU:HB2	2:C:168:ARG:HG3	1.68	0.74
2:M:628:PHE:H	2:M:638:ASP:HB3	1.51	0.74
2:C:168:ARG:HD3	2:C:268:ASP:HB3	1.69	0.73
2:M:428:ARG:NH2	2:M:447:ALA:O	2.22	0.72
3:N:351:MET:HG2	3:N:370:ALA:HB2	1.72	0.72
2:C:711:GLU:HG2	2:C:822:VAL:HG22	1.73	0.71
3:N:1495:ILE:HD13	4:O:80:VAL:HG21	1.73	0.71
3:N:1495:ILE:HG12	4:O:88:GLU:HG3	1.72	0.70
3:D:1108:ARG:NH2	3:D:1198:TYR:O	2.25	0.69
2:C:28:ARG:HH22	2:C:42:VAL:HG21	1.58	0.69
3:N:1461:GLY:O	3:N:1465:ASN:ND2	2.26	0.68
2:C:674:VAL:HG12	2:C:869:VAL:HB	1.76	0.68
5:F:273:ARG:HG2	5:F:276:ARG:HH12	1.58	0.68
3:N:218:LYS:HG2	3:N:338:GLU:HG2	1.77	0.67
2:C:605:LYS:HB2	2:C:612:VAL:HB	1.75	0.66
3:N:1108:ARG:NH2	3:N:1198:TYR:O	2.28	0.66
3:N:124:GLU:OE2	3:N:587:ARG:NH2	2.29	0.66
3:D:256:GLU:HG3	3:D:300:LYS:HG3	1.79	0.65
3:D:208:PRO:HA	3:D:390:PRO:HA	1.78	0.64
2:C:541:SER:O	2:C:545:ASN:ND2	2.27	0.64
1:K:222:LEU:HD22	1:L:215:VAL:HG23	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:106:PRO:HG3	1:K:134:GLU:HG2	1.78	0.64
5:F:392:VAL:HG11	5:F:396:ARG:HD3	1.79	0.64
1:L:176:ARG:NH2	3:N:888:GLU:OE1	2.30	0.64
3:D:415:VAL:HG13	3:D:419:ASP:HB2	1.80	0.64
3:N:167:GLU:OE2	3:N:198:ARG:NH1	2.30	0.64
2:M:24:GLU:OE2	2:M:27:ARG:NH2	2.31	0.64
7:R:18:DG:H2''	7:R:19:DA:H5'	1.80	0.64
2:M:1100:GLN:HG3	3:N:9:ARG:HH21	1.62	0.63
2:M:343:GLN:HG3	2:M:385:PHE:HB2	1.80	0.63
3:N:970:LYS:HD3	3:N:995:LEU:HD13	1.79	0.63
5:F:279:GLN:HB3	5:F:286:PRO:HD3	1.80	0.63
2:M:290:LEU:HD22	2:M:302:VAL:HG11	1.80	0.63
3:N:260:GLU:OE1	3:N:273:ARG:NH1	2.32	0.63
3:D:127:LEU:HA	3:D:457:GLY:HA2	1.81	0.62
3:D:124:GLU:OE2	3:D:587:ARG:NH2	2.32	0.62
2:M:939:ARG:HG2	2:M:982:PRO:HD3	1.80	0.62
3:N:171:LEU:HD12	3:N:390:PRO:HG2	1.81	0.62
2:C:939:ARG:HG2	2:C:982:PRO:HD3	1.80	0.62
2:C:408:ARG:NH2	2:C:456:ALA:O	2.32	0.62
2:M:727:PRO:HB3	2:M:783:ARG:HD3	1.82	0.61
3:N:208:PRO:HA	3:N:390:PRO:HA	1.82	0.61
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.81	0.61
3:N:643:GLY:HA3	3:N:727:GLN:HB2	1.83	0.61
1:L:56:VAL:HG22	1:L:142:VAL:HG12	1.83	0.61
2:C:324:ASP:HB3	2:C:327:HIS:HB2	1.82	0.61
1:A:106:PRO:HG3	1:A:134:GLU:HG2	1.82	0.61
3:D:356:PRO:HG2	3:D:359:ALA:HB2	1.82	0.60
2:M:740:GLU:OE1	2:M:805:ARG:NH1	2.34	0.60
2:M:420:ARG:NH2	5:P:324:GLU:OE2	2.35	0.60
5:P:365:GLU:HB2	5:P:404:ALA:HB2	1.84	0.60
1:A:55:SER:HB3	1:A:143:ARG:HB3	1.82	0.60
3:N:65:ARG:NH1	5:P:378:GLY:O	2.35	0.60
3:N:356:PRO:HG2	3:N:359:ALA:HB2	1.83	0.59
2:C:715:THR:OG1	2:C:718:GLY:O	2.19	0.59
3:D:260:GLU:OE1	3:D:273:ARG:NH1	2.35	0.59
2:C:586:ARG:NH2	2:C:590:ASP:OD1	2.36	0.59
5:F:193:ARG:HB2	6:H:6:DT:H1'	1.84	0.59
3:N:366:LYS:HD3	3:N:369:ALA:HB2	1.84	0.59
2:C:637:LEU:HG	2:C:659:PRO:HG3	1.83	0.59
4:O:39:VAL:O	4:O:72:ARG:NH1	2.31	0.59
2:C:462:ASP:OD2	2:C:468:ARG:NH1	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:266:ARG:NH1	6:H:11:DG:O6	2.35	0.59
3:N:128:TYR:OH	3:N:579:ASP:OD2	2.20	0.59
3:N:569:ASN:ND2	5:P:214:GLN:OE1	2.35	0.59
2:C:64:LEU:HD12	2:C:103:LYS:HB2	1.85	0.59
3:D:685:ASP:HA	3:D:688:TRP:HD1	1.66	0.59
3:D:1461:GLY:O	3:D:1465:ASN:ND2	2.36	0.58
2:C:758:ARG:HH21	2:C:788:THR:HB	1.67	0.58
3:D:954:ALA:O	3:D:1062:ARG:NH2	2.35	0.58
1:A:58:ILE:HG12	1:A:140:MET:HG2	1.85	0.58
3:D:1236:LEU:HA	3:D:1359:GLN:HG3	1.85	0.58
2:C:232:GLU:HG3	2:C:250:ARG:HE	1.69	0.58
1:A:218:LEU:HD23	1:B:222:LEU:HD21	1.85	0.58
3:D:273:ARG:HB3	3:D:278:PRO:HA	1.86	0.58
2:M:807:ARG:NH1	13:M:1205:HOH:O	2.37	0.58
3:N:704:ARG:NH2	10:N:1605:C:O2'	2.36	0.58
5:P:270:LYS:HG2	5:P:295:MET:HE1	1.84	0.58
2:C:172:ILE:HG12	2:C:186:VAL:HG22	1.86	0.58
2:C:202:TYR:OH	2:C:300:ASP:OD1	2.20	0.58
2:C:710:ILE:HD12	2:C:790:LEU:HB2	1.85	0.58
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.85	0.58
3:D:787:LEU:HD21	3:D:947:ILE:HG21	1.85	0.57
2:M:172:ILE:HG12	2:M:186:VAL:HG22	1.85	0.57
3:N:1047:LYS:HD3	3:N:1051:GLU:HB3	1.87	0.57
2:M:17:PRO:HB2	2:M:20:GLU:HB3	1.86	0.57
3:N:787:LEU:HD21	3:N:947:ILE:HG21	1.87	0.57
3:D:1040:GLY:O	3:D:1060:SER:HB3	2.05	0.57
2:M:92:ALA:HB2	2:M:120:LEU:HD11	1.86	0.57
5:F:131:VAL:HG13	5:F:178:ARG:HD3	1.86	0.57
3:D:996:TRP:CD2	3:D:1056:PRO:HG3	2.40	0.57
2:M:324:ASP:O	2:M:330:ASN:ND2	2.29	0.57
2:C:283:ILE:HD13	2:C:305:PRO:HG2	1.86	0.56
3:D:657:LEU:HG	3:D:661:MET:HE2	1.86	0.56
2:C:12:VAL:HG13	2:C:13:ILE:HG23	1.87	0.56
3:N:474:GLU:HG3	3:N:496:LEU:HD11	1.88	0.56
1:L:11:PHE:HE1	1:L:23:PHE:HB3	1.69	0.56
1:B:92:PRO:O	1:B:146:ARG:NH2	2.39	0.56
5:P:210:LEU:HD23	5:P:213:ILE:HD12	1.87	0.56
1:K:222:LEU:HD21	1:L:218:LEU:HD23	1.89	0.55
5:P:131:VAL:HG13	5:P:178:ARG:HD3	1.88	0.55
2:M:768:THR:OG1	2:M:771:GLU:OE1	2.25	0.55
3:D:474:GLU:HG3	3:D:496:LEU:HD11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:188:ILE:HD13	5:P:221:ILE:HG12	1.88	0.55
2:C:428:ARG:NH2	2:C:447:ALA:O	2.32	0.55
5:F:360:LYS:HG3	5:F:411:HIS:HB2	1.88	0.55
3:N:266:GLU:HG3	3:N:314:PRO:HB3	1.88	0.55
3:N:1296:SER:HB3	3:N:1299:PHE:HB2	1.88	0.55
5:P:120:THR:HG22	5:P:122:LEU:HD13	1.90	0.54
2:C:24:GLU:HG3	2:C:27:ARG:HH22	1.72	0.54
2:C:399:ASN:O	2:C:402:SER:OG	2.22	0.54
2:M:207:LEU:HD13	2:M:221:LEU:HD21	1.89	0.54
1:A:24:VAL:HG22	1:A:196:THR:HG23	1.88	0.54
5:F:284:ARG:NH2	5:F:290:GLU:OE2	2.38	0.54
2:C:207:LEU:HD13	2:C:221:LEU:HD21	1.89	0.54
2:M:168:ARG:HA	2:M:168:ARG:HE	1.73	0.54
3:D:1495:ILE:HG21	4:E:80:VAL:HG12	1.90	0.54
3:D:904:VAL:HG22	3:D:905:PRO:HD2	1.89	0.54
3:N:703:ASN:HB2	3:N:713:ILE:HG12	1.89	0.54
3:D:1042:ARG:HB3	3:D:1057:VAL:HB	1.90	0.54
3:D:266:GLU:HG3	3:D:314:PRO:HB3	1.90	0.54
3:D:658:LEU:HA	3:D:661:MET:HE3	1.88	0.54
1:L:80:LEU:HD21	3:N:842:VAL:HG12	1.90	0.54
3:D:734:GLU:OE2	3:D:780:LYS:NZ	2.40	0.54
3:N:1152:GLU:HG2	3:N:1162:GLU:H	1.72	0.54
3:N:172:PRO:HG2	3:N:175:VAL:HB	1.90	0.53
1:B:108:GLU:HG2	1:B:131:THR:HG22	1.89	0.53
2:C:714:ASP:OD2	2:C:808:ARG:NH1	2.41	0.53
3:D:1020:LEU:HB3	3:D:1035:ILE:HD12	1.89	0.53
3:D:563:PRO:HD2	3:D:566:ILE:HD12	1.89	0.53
3:N:685:ASP:HA	3:N:688:TRP:HD1	1.72	0.53
2:C:39:ARG:NH1	2:C:71:TYR:O	2.29	0.53
3:D:231:VAL:O	3:D:236:TYR:OH	2.26	0.53
2:C:55:GLU:O	2:C:356:ARG:NH2	2.41	0.53
3:D:1047:LYS:HD3	3:D:1051:GLU:HG3	1.90	0.53
3:D:1044:LEU:HD23	3:D:1056:PRO:HB3	1.90	0.53
3:D:242:LEU:HB3	3:D:311:LEU:HD12	1.89	0.53
3:D:707:THR:HG23	3:D:712:GLY:HA3	1.91	0.53
5:F:120:THR:HG22	5:F:122:LEU:HD13	1.91	0.53
2:M:283:ILE:HD13	2:M:305:PRO:HG2	1.91	0.53
2:M:758:ARG:HH21	2:M:788:THR:HB	1.72	0.53
3:N:353:VAL:HG11	3:N:387:LEU:HD11	1.90	0.53
1:B:56:VAL:HG22	1:B:142:VAL:HG12	1.90	0.53
2:C:754:ILE:HG12	2:C:791:ARG:HG2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:238:PRO:HD3	3:N:318:ARG:HG2	1.89	0.53
2:C:900:ARG:NH1	13:C:1206:HOH:O	2.42	0.53
3:D:809:PRO:HB3	3:D:839:LEU:HD13	1.90	0.53
3:N:644:LEU:HD12	3:N:645:PRO:HD2	1.89	0.53
3:D:520:LEU:O	3:D:525:ARG:NE	2.39	0.53
2:M:1110:ASP:OD2	2:M:1114:GLY:N	2.33	0.53
2:C:370:ALA:O	5:F:280:GLN:NE2	2.38	0.53
2:M:462:ASP:HB3	2:M:468:ARG:HD2	1.91	0.53
1:K:59:GLU:OE1	1:K:139:ASN:ND2	2.37	0.53
3:N:1044:LEU:HD23	3:N:1056:PRO:HB3	1.90	0.53
2:M:937:ASP:OD1	2:M:939:ARG:HD3	2.09	0.52
3:N:132:TYR:OH	3:N:568:ARG:NH1	2.43	0.52
2:C:1019:GLN:HG2	2:C:1058:ASP:HB3	1.91	0.52
5:F:188:ILE:HG12	5:F:224:VAL:HG21	1.90	0.52
2:M:413:LEU:HD21	2:M:451:LEU:HD13	1.90	0.52
2:M:715:THR:OG1	2:M:718:GLY:O	2.23	0.52
3:N:1003:VAL:HG21	3:N:1041:LEU:HG	1.91	0.52
2:C:1038:TRP:CE2	3:D:1099:VAL:HG11	2.44	0.52
2:M:936:VAL:HG11	2:M:959:PRO:HB2	1.91	0.52
3:N:351:MET:HG2	3:N:370:ALA:CB	2.39	0.52
2:C:254:VAL:O	2:C:258:TYR:HB3	2.10	0.52
2:M:13:ILE:HD13	2:M:483:VAL:HG11	1.91	0.52
2:C:950:LEU:HB3	2:C:952:LEU:HD13	1.90	0.52
3:D:114:THR:HG23	3:D:495:ARG:HG2	1.91	0.52
3:N:356:PRO:HB3	3:N:441:ARG:HA	1.92	0.52
2:C:936:VAL:HG11	2:C:959:PRO:HB2	1.92	0.52
2:C:413:LEU:HD21	2:C:451:LEU:HD13	1.92	0.51
2:C:504:GLU:HG2	2:C:509:ALA:HB2	1.91	0.51
5:F:361:LEU:HD13	5:F:407:LYS:HD2	1.92	0.51
1:L:108:GLU:HG2	1:L:131:THR:HG22	1.92	0.51
2:M:571:LEU:HB2	2:M:574:ALA:HB2	1.92	0.51
3:N:1374:GLN:NE2	13:N:2104:HOH:O	2.42	0.51
2:C:657:ASP:OD2	2:C:663:ASN:N	2.44	0.51
3:N:956:ILE:HD11	3:N:1062:ARG:HG2	1.90	0.51
3:N:575:GLN:NE2	3:N:579:ASP:OD1	2.43	0.51
2:M:160:ALA:HB3	2:M:174:LEU:HB2	1.92	0.51
5:F:370:LYS:HG2	5:F:375:LEU:HD22	1.93	0.51
3:N:1101:VAL:HG13	3:N:1102:THR:HG23	1.91	0.51
3:D:1350:GLU:OE2	3:D:1357:ARG:NH1	2.40	0.51
3:D:256:GLU:HG2	3:D:299:GLU:HA	1.92	0.51
3:D:647:ARG:HH21	3:D:724:GLN:HG2	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:41:ASN:O	2:M:46:ALA:HB2	2.11	0.51
3:N:633:VAL:HB	3:N:740:PHE:CE2	2.45	0.51
2:C:460:ARG:HD3	2:C:485:TYR:CE2	2.46	0.51
2:C:971:LYS:HB3	2:C:986:PRO:HB2	1.93	0.51
1:B:176:ARG:NH2	3:D:888:GLU:OE1	2.44	0.51
3:D:1101:VAL:HG13	3:D:1102:THR:HG23	1.93	0.51
7:G:14:DA:H2'	7:G:15:DG:C8	2.45	0.51
3:N:1236:LEU:HA	3:N:1359:GLN:HG3	1.93	0.51
3:N:895:VAL:HG11	3:N:922:LEU:HD21	1.93	0.51
2:C:800:VAL:HG22	2:C:827:VAL:HG22	1.92	0.51
3:D:956:ILE:HD11	3:D:1062:ARG:HG2	1.93	0.51
2:M:1008:ARG:NH2	13:M:1203:HOH:O	2.33	0.51
3:N:455:ARG:HB2	3:N:460:ALA:HB2	1.92	0.51
2:C:168:ARG:O	2:C:267:TYR:HA	2.11	0.50
2:M:1038:TRP:CE2	3:N:1099:VAL:HG11	2.46	0.50
2:M:847:GLY:HA2	3:N:741:ASP:HA	1.93	0.50
5:F:152:ASP:OD1	5:F:152:ASP:N	2.43	0.50
2:M:711:GLU:HG2	2:M:822:VAL:HG22	1.92	0.50
2:M:787:ASP:OD2	2:M:791:ARG:NH2	2.40	0.50
1:B:80:LEU:HD21	3:D:842:VAL:HG12	1.93	0.50
3:D:1068:LEU:O	3:D:1072:ILE:HG12	2.12	0.50
5:P:188:ILE:HG12	5:P:224:VAL:HG21	1.94	0.50
3:N:809:PRO:HB3	3:N:839:LEU:HD13	1.93	0.50
5:F:135:ILE:HG13	5:F:181:GLU:HB2	1.93	0.50
3:N:840:LYS:HE3	3:N:841:TYR:CZ	2.47	0.50
3:N:314:PRO:HB2	3:N:317:VAL:HG12	1.94	0.50
2:C:712:ALA:HB3	2:C:821:GLU:HG3	1.94	0.50
2:C:808:ARG:NH2	5:F:305:GLU:OE2	2.45	0.49
3:D:407:VAL:HG22	3:D:409:VAL:H	1.77	0.49
2:M:670:GLN:HG2	2:M:699:PHE:CD2	2.47	0.49
3:N:899:LEU:HD22	3:N:917:GLN:HB3	1.93	0.49
2:C:122:THR:HG22	2:C:123:GLU:H	1.76	0.49
1:K:196:THR:HG21	2:M:934:PHE:HE1	1.77	0.49
3:N:637:LEU:HD13	3:N:642:CYS:HA	1.94	0.49
2:C:111:ASP:OD1	2:C:112:GLU:N	2.45	0.49
2:C:223:ASP:OD1	2:C:225:SER:OG	2.25	0.49
2:C:513:VAL:HG13	2:C:524:VAL:HG23	1.94	0.49
3:D:192:ALA:HB3	3:D:195:VAL:HB	1.95	0.49
3:N:890:VAL:HB	3:N:922:LEU:HD13	1.93	0.49
2:M:1067:TYR:OH	3:N:674:ARG:NH1	2.42	0.49
2:M:168:ARG:O	2:M:267:TYR:HA	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:285:LEU:HD21	2:C:302:VAL:HG22	1.95	0.49
3:N:500:ARG:NH1	3:N:1388:ARG:O	2.44	0.49
3:D:241:ILE:HG12	3:D:310:LEU:HD21	1.95	0.49
2:M:843:HIS:NE2	2:M:887:GLU:OE2	2.41	0.49
1:A:36:LEU:HD11	1:B:221:HIS:HB3	1.95	0.49
2:C:331:ARG:NH1	13:C:1205:HOH:O	2.37	0.49
1:A:65:PHE:HE1	2:C:703:ILE:HD12	1.78	0.49
3:D:664:LYS:HB2	3:D:666:ILE:HD12	1.94	0.49
3:N:975:GLU:O	3:N:979:GLU:HG2	2.12	0.49
1:A:6:LEU:HD11	1:A:27:PRO:HG2	1.95	0.48
2:M:1009:SER:HB3	3:N:651:GLU:O	2.12	0.48
2:C:299:LYS:HE3	2:C:300:ASP:H	1.77	0.48
2:M:390:GLN:HB3	2:M:415:PRO:HD3	1.96	0.48
3:D:261:LEU:HD13	3:D:270:LEU:HD12	1.95	0.48
2:C:886:LEU:HD21	3:D:951:ILE:HG12	1.95	0.48
2:M:229:MET:HB2	2:M:233:GLU:HB2	1.96	0.48
2:M:674:VAL:HG12	2:M:869:VAL:HB	1.96	0.48
2:C:164:PRO:HA	2:C:269:LEU:HD23	1.95	0.48
2:C:390:GLN:HG2	2:C:414:GLY:HA2	1.94	0.48
5:F:153:PRO:HA	5:F:156:VAL:HG22	1.96	0.48
2:M:223:ASP:OD1	2:M:225:SER:OG	2.26	0.48
3:N:106:LYS:O	3:N:586:ARG:NH1	2.46	0.48
3:N:1068:LEU:O	3:N:1072:ILE:HG12	2.13	0.48
3:N:192:ALA:HB3	3:N:195:VAL:HB	1.96	0.48
2:C:937:ASP:OD1	2:C:939:ARG:HD3	2.14	0.48
10:N:1605:C:O2	7:R:15:DG:N2	2.37	0.48
2:C:32:ALA:HB2	2:C:73:LEU:HD12	1.95	0.48
2:M:911:GLU:O	2:M:915:LYS:HG2	2.14	0.48
1:A:179:PHE:HB3	1:A:197:LEU:HD23	1.96	0.48
1:K:25:LEU:HD23	1:K:28:LEU:HD11	1.96	0.48
1:L:92:PRO:O	1:L:146:ARG:NH2	2.46	0.48
3:N:162:ARG:O	3:N:449:SER:HB2	2.14	0.48
2:C:41:ASN:O	2:C:46:ALA:HB2	2.14	0.48
3:D:50:PHE:O	3:D:89:ARG:HD2	2.14	0.48
1:B:38:ASN:ND2	2:C:978:ARG:O	2.46	0.48
3:D:272:LEU:HB2	3:D:280:ALA:HB3	1.96	0.48
2:C:87:ASP:HA	2:C:131:GLY:HA3	1.96	0.47
2:M:281:LEU:HD13	2:M:305:PRO:HB2	1.96	0.47
3:N:307:ALA:HB1	3:N:311:LEU:HD11	1.96	0.47
5:F:370:LYS:HB3	5:F:375:LEU:HB2	1.96	0.47
2:C:324:ASP:O	2:C:330:ASN:ND2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:383:LEU:H	5:F:383:LEU:HD22	1.79	0.47
2:M:711:GLU:O	2:M:758:ARG:NH1	2.46	0.47
3:N:1353:GLN:NE2	3:N:1365:ASP:OD1	2.46	0.47
5:P:93:LEU:HD21	5:P:193:ARG:HD2	1.95	0.47
1:K:179:PHE:HB3	1:K:197:LEU:HD23	1.96	0.47
2:C:599:GLU:HG3	2:C:600:ASP:H	1.79	0.47
1:L:83:LYS:HE2	1:L:168:ASP:HB2	1.95	0.47
1:L:8:ALA:HB1	1:L:9:PRO:HA	1.97	0.47
1:A:64:GLU:HG2	1:A:76:VAL:HG22	1.96	0.47
1:K:216:GLU:OE2	1:K:219:ARG:NH2	2.48	0.47
3:N:368:VAL:HB	3:N:377:VAL:HB	1.96	0.47
5:P:212:LEU:HD22	5:P:247:ILE:HG23	1.95	0.47
2:C:261:ILE:HD11	2:C:303:PHE:CZ	2.48	0.47
2:C:773:LEU:HD23	5:F:354:LEU:HD13	1.96	0.47
3:N:1105:ILE:HG23	3:N:1199:GLY:HA2	1.96	0.47
2:M:1104:GLU:HG2	3:N:6:ARG:HG3	1.97	0.47
3:N:954:ALA:O	3:N:1062:ARG:NH2	2.47	0.47
5:P:144:ILE:HB	5:P:147:LEU:HD13	1.96	0.47
2:C:470:PRO:HG3	2:C:485:TYR:CE2	2.50	0.47
3:D:1147:ARG:NH2	3:D:1369:GLU:OE1	2.43	0.47
3:D:97:THR:HG21	3:D:571:LYS:HG2	1.96	0.47
2:M:740:GLU:HB3	2:M:805:ARG:HH12	1.79	0.47
3:N:166:GLN:HB3	3:N:396:VAL:HG13	1.97	0.47
3:D:1285:GLU:HG3	3:D:1290:LEU:HG	1.97	0.47
1:K:218:LEU:HD23	1:L:222:LEU:HD21	1.96	0.47
1:A:210:ALA:HA	1:A:213:GLN:HE21	1.80	0.46
3:D:417:PRO:HG3	3:D:431:VAL:HA	1.97	0.46
1:L:128:HIS:CE1	1:L:131:THR:HG23	2.51	0.46
3:N:797:LYS:HE3	3:N:826:PRO:HG3	1.98	0.46
3:D:162:ARG:O	3:D:449:SER:HB2	2.15	0.46
2:M:617:ASP:HB2	2:M:619:ARG:HG2	1.97	0.46
3:D:1168:MET:HA	3:D:1168:MET:HE3	1.98	0.46
5:F:386:VAL:HG13	5:F:397:ILE:HG21	1.98	0.46
3:D:750:PRO:HG2	3:D:756:GLN:NE2	2.30	0.46
1:A:57:TYR:HE1	1:A:163:ASN:HB2	1.81	0.46
2:C:390:GLN:HB3	2:C:415:PRO:HD3	1.97	0.46
5:F:414:ARG:HG2	5:F:415:THR:HG23	1.98	0.46
2:C:267:TYR:CE1	2:C:290:LEU:HG	2.50	0.46
5:F:412:GLU:O	5:F:416:ARG:N	2.43	0.46
1:K:209:GLU:O	1:K:213:GLN:HG2	2.16	0.46
1:K:24:VAL:HG22	1:K:196:THR:HG23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:55:SER:HB3	1:L:143:ARG:HB3	1.96	0.46
3:N:822:ALA:HB3	3:N:825:ALA:HB2	1.98	0.46
2:C:105:THR:HG22	2:C:107:LEU:H	1.81	0.46
1:K:26:GLU:HB3	1:K:194:LYS:HG3	1.97	0.46
2:M:1095:LEU:HD23	3:N:582:LEU:HD22	1.98	0.46
3:N:606:ILE:O	3:N:613:ARG:N	2.49	0.46
3:D:1379:VAL:HG21	3:D:1400:VAL:HG11	1.98	0.46
5:F:392:VAL:HG12	5:F:393:THR:H	1.81	0.46
2:M:419:THR:HG23	2:M:422:ARG:HG3	1.98	0.45
3:N:1102:THR:HG21	3:N:1371:VAL:HG22	1.98	0.45
3:N:707:THR:HG23	3:N:712:GLY:HA3	1.99	0.45
2:C:470:PRO:HB2	2:C:534:VAL:HG21	1.98	0.45
1:K:70:GLY:N	2:M:607:ASP:OD1	2.50	0.45
3:N:850:LEU:HD12	3:N:884:ARG:NH2	2.31	0.45
5:P:373:LYS:HD3	5:P:373:LYS:HA	1.85	0.45
3:D:487:ALA:O	3:D:491:LYS:HG2	2.16	0.45
3:D:633:VAL:C	3:D:635:PRO:HD3	2.37	0.45
5:F:93:LEU:HD21	5:F:193:ARG:HD2	1.97	0.45
3:D:356:PRO:HB3	3:D:441:ARG:HA	1.99	0.45
3:D:834:THR:OG1	3:D:835:SER:N	2.49	0.45
3:N:224:ARG:NE	3:N:254:GLU:OE2	2.40	0.45
1:B:77:GLU:OE1	3:D:867:ARG:NH2	2.44	0.45
3:D:1364:HIS:ND1	3:D:1366:LYS:HG2	2.32	0.45
3:D:22:SER:HB2	3:D:92:HIS:HB3	1.99	0.45
1:A:216:GLU:OE2	1:A:219:ARG:NH2	2.50	0.45
3:D:101:HIS:HB3	3:D:104:PHE:HD2	1.82	0.45
1:K:133:GLU:HG2	1:K:134:GLU:H	1.81	0.45
3:N:1216:SER:N	13:N:2117:HOH:O	2.50	0.45
5:P:80:PRO:HB2	5:P:210:LEU:HD11	1.99	0.45
3:D:248:PRO:HG3	3:D:308:LYS:HE3	1.98	0.45
3:D:314:PRO:HB2	3:D:317:VAL:HG12	1.98	0.45
1:L:90:LEU:HD13	1:L:90:LEU:HA	1.75	0.45
2:M:324:ASP:HB3	2:M:327:HIS:HB2	1.99	0.45
2:M:390:GLN:HG2	2:M:414:GLY:HA2	1.98	0.45
2:M:504:GLU:HG2	2:M:509:ALA:HB2	1.99	0.45
2:M:425:PHE:CE1	3:N:1086:LEU:HD12	2.52	0.45
5:P:187:LEU:HD23	5:P:224:VAL:HG13	1.97	0.45
3:D:890:VAL:HG23	3:D:892:ASP:H	1.81	0.45
3:N:633:VAL:O	3:N:635:PRO:HD3	2.17	0.45
5:P:193:ARG:HB2	6:S:6:DT:H1'	1.98	0.45
3:D:285:PRO:HD2	3:D:288:MET:SD	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:205:ARG:HG3	5:F:251:ILE:HD13	1.99	0.45
2:M:708:TYR:HB3	2:M:790:LEU:HD21	1.99	0.45
2:M:950:LEU:HB3	2:M:952:LEU:HD13	1.99	0.44
3:N:685:ASP:HA	3:N:688:TRP:CD1	2.52	0.44
5:P:153:PRO:HA	5:P:156:VAL:HG22	1.98	0.44
2:C:1009:SER:HB3	3:D:651:GLU:O	2.17	0.44
2:C:469:THR:HA	2:C:470:PRO:HD3	1.88	0.44
3:D:67:ARG:CZ	5:F:379:ARG:HD2	2.47	0.44
1:K:53:VAL:HG22	1:K:144:VAL:HG22	1.99	0.44
2:M:678:PRO:HA	2:M:683:ASN:HD21	1.82	0.44
3:N:657:LEU:HG	3:N:661:MET:HE2	2.00	0.44
3:N:629:SER:HB3	3:N:726:ILE:HG13	1.99	0.44
5:P:193:ARG:HB3	6:S:7:DG:H5''	1.98	0.44
3:D:1500:LYS:HB3	3:D:1500:LYS:HE2	1.79	0.44
6:H:10:DA:H2''	6:H:11:DG:C8	2.53	0.44
3:N:407:VAL:HG22	3:N:409:VAL:H	1.81	0.44
3:N:42:ASP:OD1	3:N:48:ARG:NH1	2.50	0.44
2:C:353:ARG:NH2	5:F:203:THR:OG1	2.50	0.44
3:D:644:LEU:HD12	3:D:645:PRO:HD2	1.98	0.44
1:L:77:GLU:OE1	3:N:867:ARG:NH2	2.41	0.44
2:M:535:SER:O	2:M:538:GLN:HG2	2.17	0.44
5:P:234:LYS:HG3	6:S:4:DA:H3'	1.99	0.44
3:D:397:LYS:HB3	3:D:397:LYS:HE2	1.86	0.44
2:M:177:GLU:HG3	2:M:178:PRO:HD2	2.00	0.44
2:M:40:GLU:O	2:M:45:GLN:HG2	2.17	0.44
2:M:607:ASP:HB2	2:M:610:ARG:HH11	1.82	0.44
3:D:14:SER:HB3	3:D:511:TRP:CE2	2.52	0.44
3:D:864:VAL:HG22	3:D:865:THR:H	1.83	0.44
1:A:53:VAL:HG22	1:A:144:VAL:HG22	2.00	0.44
2:C:22:GLN:HG3	2:C:407:LYS:HB3	2.00	0.44
3:D:171:LEU:HD12	3:D:390:PRO:HG2	2.00	0.44
3:D:371:ILE:HG23	5:F:230:LYS:HD2	1.99	0.44
1:L:111:ALA:HB3	1:L:125:PRO:HA	1.98	0.44
2:M:610:ARG:HG2	2:M:611:ILE:N	2.33	0.44
2:C:1110:ASP:OD2	2:C:1114:GLY:N	2.32	0.43
2:C:684:PHE:HB3	3:D:633:VAL:HG21	2.00	0.43
3:D:520:LEU:HD12	3:D:521:PRO:HD2	2.00	0.43
3:D:555:LYS:HA	5:F:142:ARG:HH12	1.83	0.43
1:K:150:TYR:CD1	2:M:696:LYS:HG2	2.53	0.43
2:M:605:LYS:HB2	2:M:612:VAL:HB	1.99	0.43
3:N:1377:LYS:HE3	3:N:1378:TYR:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1071:PHE:O	3:D:1074:SER:OG	2.35	0.43
3:D:1283:ILE:HG13	3:D:1283:ILE:H	1.70	0.43
6:H:16:DC:H2"	6:H:17:DA:H5'	1.99	0.43
1:K:91:ASN:HA	1:K:92:PRO:HD3	1.85	0.43
3:N:101:HIS:HB3	3:N:104:PHE:HD2	1.82	0.43
5:P:163:LEU:HD13	5:P:174:LEU:HD13	2.00	0.43
1:B:64:GLU:HA	1:B:165:ILE:HD13	2.01	0.43
3:D:39:PRO:HG2	3:D:47:GLU:HG3	2.00	0.43
2:C:766:GLU:HG2	3:D:65:ARG:HE	1.83	0.43
3:N:619:LEU:HD11	3:N:1439:SER:HB2	2.00	0.43
3:N:569:ASN:O	3:N:573:MET:HG3	2.19	0.43
5:P:279:GLN:HB3	5:P:286:PRO:HD3	1.99	0.43
1:L:71:VAL:HG22	1:L:132:LEU:HG	2.00	0.43
2:M:675:ALA:HB2	2:M:867:VAL:HG11	1.99	0.43
3:N:864:VAL:HG22	3:N:865:THR:H	1.82	0.43
1:A:102:LYS:HB2	1:A:102:LYS:HE3	1.89	0.43
1:A:112:ARG:HG3	1:A:125:PRO:HB2	2.01	0.43
3:D:200:ASP:O	3:D:397:LYS:HG2	2.17	0.43
3:D:610:LYS:HA	3:D:615:ARG:HD3	2.00	0.43
2:C:389:SER:OG	2:C:390:GLN:N	2.52	0.43
2:C:1051:GLU:HG3	2:C:1055:LEU:HD12	2.01	0.43
3:D:1381:VAL:HG21	3:D:1389:LEU:HD23	1.99	0.43
3:D:142:LEU:HB2	3:D:161:LEU:HD11	2.00	0.43
4:E:40:LEU:HG	4:E:67:GLU:HG2	2.01	0.43
5:F:144:ILE:HB	5:F:147:LEU:HD13	2.00	0.43
5:F:270:LYS:HG2	5:F:295:MET:HE1	2.01	0.43
5:F:414:ARG:HG2	5:F:415:THR:N	2.34	0.43
3:N:472:ALA:O	3:N:476:GLU:HG2	2.18	0.43
3:N:114:THR:HG23	3:N:495:ARG:HG2	2.01	0.43
2:C:12:VAL:HG11	2:C:472:ARG:HD3	2.01	0.43
2:C:584:GLU:N	2:C:584:GLU:OE2	2.52	0.43
4:E:83:ASP:O	4:E:87:LYS:HG2	2.19	0.43
5:F:323:ASP:N	5:F:323:ASP:OD1	2.52	0.43
4:E:13:VAL:HG21	4:E:19:LEU:HB2	2.00	0.43
2:M:210:GLU:HG2	2:M:304:LEU:HD21	2.00	0.43
3:N:483:HIS:CG	3:N:484:PRO:HD2	2.53	0.43
5:P:323:ASP:N	5:P:323:ASP:OD1	2.31	0.43
1:A:133:GLU:HG2	1:A:134:GLU:H	1.84	0.42
1:A:209:GLU:O	1:A:213:GLN:HG2	2.19	0.42
1:B:124:ASN:N	1:B:124:ASN:OD1	2.52	0.42
1:B:150:TYR:CE2	1:B:170:VAL:HG22	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:187:LYS:N	3:D:200:ASP:OD2	2.43	0.42
3:D:236:TYR:HB3	3:D:313:MET:HG3	2.01	0.42
3:D:729:HIS:HA	3:D:730:PRO:HD3	1.93	0.42
3:D:741:ASP:N	3:D:741:ASP:OD1	2.48	0.42
3:D:935:LYS:HB3	3:D:935:LYS:HE2	1.88	0.42
1:K:87:VAL:HG21	1:K:144:VAL:HG21	2.00	0.42
2:M:848:VAL:HG22	3:N:740:PHE:O	2.19	0.42
1:A:226:SER:O	1:A:228:PRO:HD3	2.19	0.42
2:C:146:VAL:HG21	2:C:281:LEU:HD11	2.01	0.42
2:C:249:LYS:HE2	2:C:249:LYS:HB3	1.85	0.42
2:C:911:GLU:O	2:C:915:LYS:HG2	2.19	0.42
2:M:35:PRO:HA	2:M:36:PRO:HD3	1.89	0.42
3:N:137:PRO:HD3	3:N:149:LYS:HG3	2.01	0.42
3:N:715:ALA:HB3	3:N:764:LEU:HA	2.00	0.42
5:P:285:GLU:HA	5:P:286:PRO:HD3	1.81	0.42
1:B:94:LEU:O	1:B:146:ARG:NH2	2.49	0.42
2:C:247:PRO:HA	2:C:248:PRO:HD3	1.75	0.42
3:D:1124:GLN:OE1	3:D:1133:ARG:NH1	2.52	0.42
3:D:355:VAL:HG11	3:D:385:VAL:HG21	2.00	0.42
1:L:104:GLU:OE2	1:L:137:ARG:NH1	2.53	0.42
2:M:12:VAL:HG21	2:M:472:ARG:HD3	2.01	0.42
3:N:1040:GLY:O	3:N:1060:SER:HB3	2.19	0.42
3:N:1462:LEU:HD22	3:N:1472:ILE:HB	2.01	0.42
2:C:1090:LYS:HD3	2:C:1090:LYS:HA	1.86	0.42
2:C:1106:ASP:OD1	3:D:7:LYS:NZ	2.44	0.42
3:D:500:ARG:NH1	3:D:1388:ARG:O	2.41	0.42
3:D:181:ASP:HB2	3:D:205:TYR:CD2	2.54	0.42
3:D:259:VAL:HG22	3:D:272:LEU:HD11	2.01	0.42
3:D:764:LEU:O	3:D:768:ASN:ND2	2.53	0.42
2:M:879:ARG:NH1	13:M:1216:HOH:O	2.52	0.42
3:N:1344:VAL:HG11	3:N:1421:LEU:HD22	2.01	0.42
3:D:850:LEU:HD12	3:D:884:ARG:NH2	2.35	0.42
5:F:222:ARG:NH2	5:F:225:GLU:OE1	2.52	0.42
2:M:602:GLU:HB2	2:M:648:ARG:HH21	1.84	0.42
3:N:1000:THR:HG23	3:N:1036:ARG:HD2	2.01	0.42
6:S:10:DA:H2"	6:S:11:DG:C8	2.55	0.42
2:C:35:PRO:HA	2:C:36:PRO:HD3	1.90	0.42
3:D:167:GLU:OE2	3:D:198:ARG:NH1	2.53	0.42
3:D:372:ASP:HA	3:D:373:PRO:HD3	1.87	0.42
3:D:472:ALA:O	3:D:476:GLU:HG2	2.20	0.42
3:D:317:VAL:HG23	3:D:339:TRP:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:353:VAL:HG12	3:D:355:VAL:H	1.85	0.42
3:D:684:LYS:HB3	3:D:684:LYS:HE2	1.86	0.42
2:M:299:LYS:HB2	2:M:299:LYS:HE3	1.84	0.42
3:N:129:PHE:CD2	3:N:456:MET:HB3	2.54	0.42
3:N:72:VAL:HA	3:N:79:GLU:HA	2.02	0.42
5:P:333:ILE:HA	5:P:334:PRO:HD3	1.82	0.42
6:S:19:DG:H2'	6:S:20:DG:C8	2.55	0.42
2:C:631:SER:HB3	2:C:637:LEU:HD13	2.02	0.42
2:M:118:ILE:HD11	2:M:344:PHE:CE1	2.55	0.42
2:M:611:ILE:HD11	2:M:641:PRO:HB3	2.02	0.42
2:M:976:ASP:OD1	2:M:978:ARG:HD3	2.19	0.42
3:N:1115:THR:O	3:N:1151:ARG:NH1	2.53	0.42
3:N:633:VAL:HB	3:N:740:PHE:CZ	2.54	0.42
2:C:1100:GLN:HG3	3:D:9:ARG:HH21	1.85	0.42
1:L:11:PHE:CE1	1:L:23:PHE:HB3	2.52	0.42
1:L:51:THR:OG1	1:L:87:VAL:O	2.35	0.42
2:M:976:ASP:HB3	2:M:979:THR:OG1	2.20	0.42
3:N:1366:LYS:O	3:N:1370:ILE:HG12	2.19	0.42
3:N:256:GLU:OE1	3:N:274:ARG:NH1	2.53	0.42
3:N:200:ASP:O	3:N:397:LYS:HG2	2.20	0.42
3:N:1498:ALA:HB1	4:O:84:ARG:HH21	1.84	0.42
1:B:90:LEU:HA	1:B:90:LEU:HD13	1.79	0.42
1:A:180:GLN:NE2	2:C:935:GLY:O	2.53	0.42
3:D:1189:ARG:HB3	3:D:1204:CYS:HA	2.02	0.42
3:D:890:VAL:HB	3:D:922:LEU:HD13	2.02	0.42
1:K:198:ARG:HD3	2:M:934:PHE:CZ	2.55	0.42
2:M:436:GLY:HA2	2:M:538:GLN:O	2.20	0.42
3:N:1208:ASP:HB2	3:N:1215:VAL:HA	2.02	0.42
3:N:1267:ARG:HA	3:N:1268:PRO:HD3	1.92	0.42
3:N:236:TYR:CD2	3:N:322:VAL:HG21	2.55	0.42
3:N:750:PRO:HG2	3:N:756:GLN:NE2	2.35	0.42
1:A:51:THR:OG1	1:A:87:VAL:O	2.29	0.41
2:C:1009:SER:O	3:D:624:ASP:HB3	2.19	0.41
2:C:1043:TYR:CD2	3:D:763:MET:HG2	2.56	0.41
2:C:285:LEU:HB3	2:C:287:GLY:O	2.20	0.41
2:C:469:THR:HG23	2:C:471:TYR:CE2	2.55	0.41
3:D:1487:VAL:HG22	3:D:1491:THR:HB	2.02	0.41
3:D:238:PRO:HD3	3:D:318:ARG:HG3	2.01	0.41
3:D:245:LEU:HA	3:D:246:PRO:HD3	1.89	0.41
1:K:79:ILE:O	1:K:83:LYS:HG3	2.20	0.41
3:N:801:GLY:O	3:N:804:LEU:HG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:809:PRO:HG3	3:N:829:VAL:HG11	2.02	0.41
5:P:338:LEU:HA	5:P:339:PRO:HD3	1.87	0.41
5:P:367:MET:HB3	5:P:390:PHE:HZ	1.85	0.41
2:C:567:GLN:O	2:C:998:TYR:N	2.53	0.41
3:D:43:GLY:H	3:D:46:ASP:HB2	1.85	0.41
3:D:90:MET:SD	3:D:521:PRO:HD3	2.61	0.41
2:M:36:PRO:HB3	2:M:70:GLU:HB2	2.02	0.41
2:C:573:ARG:NH1	2:C:697:ARG:O	2.42	0.41
2:C:670:GLN:HE22	2:C:699:PHE:HA	1.84	0.41
5:F:276:ARG:O	5:F:279:GLN:HG3	2.20	0.41
3:N:12:LEU:HD21	3:N:104:PHE:CZ	2.54	0.41
3:N:487:ALA:O	3:N:491:LYS:HG2	2.21	0.41
1:B:104:GLU:OE2	1:B:137:ARG:NH1	2.53	0.41
2:C:1090:LYS:HE2	2:C:1112:PHE:CZ	2.55	0.41
2:C:334:ARG:NH2	2:C:342:ASP:OD2	2.54	0.41
2:C:838:LYS:HE2	2:C:997:LEU:HD12	2.00	0.41
3:D:241:ILE:HD13	3:D:310:LEU:HD11	2.01	0.41
5:P:400:ILE:HA	5:P:403:LYS:HG2	2.02	0.41
2:C:168:ARG:HE	2:C:168:ARG:HA	1.85	0.41
2:C:954:THR:HA	2:C:955:PRO:HD3	1.88	0.41
3:D:65:ARG:HA	3:D:65:ARG:HD3	1.83	0.41
2:M:470:PRO:HB2	2:M:534:VAL:HG21	2.02	0.41
3:N:1381:VAL:HG21	3:N:1389:LEU:HD23	2.03	0.41
3:N:353:VAL:HG12	3:N:355:VAL:H	1.86	0.41
2:C:642:ARG:HA	2:C:642:ARG:HD2	1.84	0.41
3:D:428:LYS:HB3	3:D:428:LYS:HE2	1.92	0.41
2:M:545:ASN:HB3	2:M:583:LEU:HD22	2.02	0.41
3:N:452:ILE:H	3:N:452:ILE:HG13	1.53	0.41
2:C:24:GLU:HG3	2:C:27:ARG:NH2	2.35	0.41
2:C:276:LYS:HB3	2:C:276:LYS:HE3	1.92	0.41
1:A:196:THR:HG21	2:C:934:PHE:HE1	1.84	0.41
3:D:1208:ASP:HB2	3:D:1215:VAL:HA	2.01	0.41
4:O:37:ASN:OD1	4:O:37:ASN:N	2.49	0.41
2:C:461:VAL:HG22	2:C:467:ILE:HG12	2.03	0.41
2:C:881:ASN:OD1	2:C:881:ASN:N	2.53	0.41
3:D:1198:TYR:OH	3:D:1432:LYS:NZ	2.47	0.41
4:E:57:ASP:HA	4:E:58:PRO:HD3	1.90	0.41
5:F:187:LEU:HD23	5:F:224:VAL:HG13	2.03	0.41
2:M:205:GLU:O	2:M:209:ARG:HG2	2.21	0.41
3:N:761:ILE:HD12	4:O:20:THR:HA	2.03	0.41
1:B:153:ALA:HA	1:B:156:HIS:NE2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:778:PHE:CD2	5:F:422:LEU:HD13	2.56	0.41
2:C:899:GLN:NE2	2:C:901:TYR:OH	2.54	0.41
1:L:216:GLU:OE1	1:L:219:ARG:NH2	2.42	0.41
2:M:172:ILE:HD11	2:M:261:ILE:HD11	2.03	0.41
3:N:293:VAL:HG22	3:N:296:GLU:HG3	2.03	0.41
3:N:879:ARG:HD3	3:N:902:LEU:O	2.21	0.41
1:B:71:VAL:HG22	1:B:132:LEU:HG	2.01	0.41
3:D:1323:GLN:HA	3:D:1324:PRO:HD3	1.94	0.41
5:F:167:PRO:O	5:F:171:LYS:N	2.53	0.41
1:K:221:HIS:HA	1:K:224:TYR:CD2	2.56	0.41
3:N:262:LYS:HE2	3:N:341:GLU:OE2	2.21	0.41
5:P:134:LYS:HA	5:P:134:LYS:HD3	1.93	0.41
1:B:111:ALA:HB3	1:B:125:PRO:HA	2.03	0.41
3:D:1092:GLY:HA3	7:G:14:DA:O4'	2.21	0.41
1:K:101:LEU:HD21	1:K:109:VAL:HG11	2.03	0.41
1:K:64:GLU:HG2	1:K:76:VAL:HG22	2.03	0.41
2:M:1090:LYS:HD3	2:M:1090:LYS:HA	1.78	0.41
3:N:1323:GLN:HA	3:N:1324:PRO:HD3	1.93	0.41
3:N:181:ASP:HB2	3:N:205:TYR:CD2	2.56	0.41
3:N:711:LEU:HD12	3:N:778:LEU:HD23	2.02	0.41
4:O:40:LEU:HG	4:O:67:GLU:HG2	2.03	0.41
3:N:1151:ARG:HA	3:N:1151:ARG:HD3	1.95	0.40
1:A:54:THR:OG1	1:A:145:ASP:OD1	2.36	0.40
2:C:512:ARG:HB2	2:C:523:ILE:HD11	2.02	0.40
3:D:323:GLU:HB2	3:D:334:THR:HB	2.02	0.40
3:D:654:LYS:O	3:D:658:LEU:HG	2.21	0.40
5:F:172:ARG:O	5:F:176:ILE:HG12	2.21	0.40
1:K:31:GLY:N	1:K:193:ASP:OD2	2.54	0.40
1:K:20:TYR:OH	1:K:198:ARG:HD2	2.20	0.40
2:M:1019:GLN:HG2	2:M:1058:ASP:HB3	2.02	0.40
4:O:83:ASP:OD1	4:O:83:ASP:N	2.55	0.40
1:B:222:LEU:HD23	1:B:222:LEU:HA	1.96	0.40
2:C:983:ILE:HG21	2:C:987:ILE:HD11	2.02	0.40
4:E:80:VAL:HG21	4:E:85:LEU:HD13	2.02	0.40
5:F:285:GLU:HA	5:F:286:PRO:HD3	1.79	0.40
5:F:402:ASN:O	5:F:406:ARG:N	2.54	0.40
2:M:118:ILE:HG12	2:M:382:ILE:HD13	2.03	0.40
3:N:192:ALA:HB1	3:N:193:PRO:HD2	2.02	0.40
3:N:255:GLU:HG2	3:N:274:ARG:HH12	1.87	0.40
4:O:3:GLU:HA	4:O:4:PRO:HD3	1.93	0.40
6:S:16:DC:H2''	6:S:17:DA:H5'	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:TYR:CG	1:B:161:ARG:HD2	2.56	0.40
1:B:90:LEU:HD21	1:B:121:GLU:HB2	2.03	0.40
2:C:499:ALA:HB2	2:C:533:ASP:HB2	2.02	0.40
3:D:233:LYS:HB2	3:D:236:TYR:CZ	2.57	0.40
3:D:431:VAL:HG21	3:D:448:GLU:HG2	2.03	0.40
5:F:326:ASP:OD1	5:F:326:ASP:N	2.54	0.40
3:N:483:HIS:CE1	3:N:488:ARG:HD3	2.56	0.40
2:C:775:ARG:HH11	2:C:782:ALA:HA	1.86	0.40
2:C:874:LEU:HD23	3:D:1023:MET:SD	2.62	0.40
2:C:716:LYS:HE3	3:D:37:LEU:HG	2.03	0.40
3:D:150:ARG:HH22	3:D:468:LEU:HD21	1.85	0.40
3:D:619:LEU:HD11	3:D:1439:SER:HB2	2.04	0.40
2:M:263:ASP:O	2:M:267:TYR:N	2.53	0.40
2:M:872:ASN:HA	2:M:873:PRO:HD2	1.95	0.40
3:N:959:GLU:OE1	3:N:959:GLU:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	229/315 (73%)	224 (98%)	5 (2%)	0	100	100
1	B	221/315 (70%)	216 (98%)	5 (2%)	0	100	100
1	K	229/315 (73%)	225 (98%)	4 (2%)	0	100	100
1	L	221/315 (70%)	217 (98%)	3 (1%)	1 (0%)	29	61
2	C	1108/1119 (99%)	1075 (97%)	33 (3%)	0	100	100
2	M	1109/1119 (99%)	1080 (97%)	29 (3%)	0	100	100
3	D	1482/1524 (97%)	1445 (98%)	37 (2%)	0	100	100
3	N	1482/1524 (97%)	1447 (98%)	35 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	334 (97%)	9 (3%)	1 (0%)	41	71
5	P	344/443 (78%)	339 (98%)	5 (2%)	0	100	100
All	All	6953/7630 (91%)	6782 (98%)	169 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	F	376	ILE
1	L	8	ALA

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	200/273 (73%)	196 (98%)	4 (2%)	55	78
1	B	196/273 (72%)	195 (100%)	1 (0%)	88	94
1	K	200/273 (73%)	199 (100%)	1 (0%)	88	94
1	L	196/273 (72%)	194 (99%)	2 (1%)	76	89
2	C	936/941 (100%)	919 (98%)	17 (2%)	59	80
2	M	937/941 (100%)	916 (98%)	21 (2%)	52	76
3	D	1253/1279 (98%)	1223 (98%)	30 (2%)	49	74
3	N	1253/1279 (98%)	1232 (98%)	21 (2%)	60	82
4	E	82/88 (93%)	79 (96%)	3 (4%)	34	65
4	O	82/88 (93%)	81 (99%)	1 (1%)	71	87
5	F	301/388 (78%)	285 (95%)	16 (5%)	22	53
5	P	301/388 (78%)	294 (98%)	7 (2%)	50	75
All	All	5937/6484 (92%)	5813 (98%)	124 (2%)	53	77

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	112	ARG
1	A	113	ASP
1	A	142	VAL
1	B	115	LEU
2	C	34	VAL
2	C	118	ILE
2	C	141	HIS
2	C	224	GLU
2	C	240	THR
2	C	250	ARG
2	C	258	TYR
2	C	299	LYS
2	C	300	ASP
2	C	360	LEU
2	C	391	LEU
2	C	405	ARG
2	C	512	ARG
2	C	610	ARG
2	C	627	ARG
2	C	640	ARG
2	C	714	ASP
3	D	3	LYS
3	D	67	ARG
3	D	71	LYS
3	D	175	VAL
3	D	270	LEU
3	D	297	ILE
3	D	452	ILE
3	D	709	HIS
3	D	741	ASP
3	D	754	PHE
3	D	784	ASP
3	D	810	GLU
3	D	894	LYS
3	D	904	VAL
3	D	971	LEU
3	D	986	ARG
3	D	1083	ASP
3	D	1129	THR
3	D	1137	ARG
3	D	1184	GLN

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Mol	Chain	Res	Type
3	D	1188	VAL
3	D	1219	GLU
3	D	1252	ILE
3	D	1286	THR
3	D	1290	LEU
3	D	1307	LYS
3	D	1488	ASP
3	D	1493	LYS
3	D	1499	ARG
3	D	1501	GLU
4	E	73	LEU
4	E	84	ARG
4	E	93	TYR
5	F	88	ILE
5	F	95	THR
5	F	97	GLU
5	F	186	HIS
5	F	295	MET
5	F	323	ASP
5	F	360	LYS
5	F	365	GLU
5	F	383	LEU
5	F	392	VAL
5	F	395	GLU
5	F	399	GLN
5	F	408	LEU
5	F	409	LYS
5	F	414	ARG
5	F	422	LEU
1	K	6	LEU
1	L	7	LYS
1	L	154	GLU
2	M	102	HIS
2	M	104	ASP
2	M	133	ASP
2	M	141	HIS
2	M	200	LEU
2	M	217	LEU
2	M	274	ARG
2	M	284	ARG
2	M	302	VAL
2	M	342	ASP

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Mol	Chain	Res	Type
2	M	388	ARG
2	M	397	GLU
2	M	419	THR
2	M	583	LEU
2	M	617	ASP
2	M	640	ARG
2	M	670	GLN
2	M	775	ARG
2	M	807	ARG
2	M	1043	TYR
2	M	1105	LYS
3	N	67	ARG
3	N	71	LYS
3	N	231	VAL
3	N	255	GLU
3	N	273	ARG
3	N	346	ARG
3	N	415	VAL
3	N	632	VAL
3	N	709	HIS
3	N	717	GLN
3	N	754	PHE
3	N	784	ASP
3	N	810	GLU
3	N	894	LYS
3	N	907	GLU
3	N	986	ARG
3	N	1067	VAL
3	N	1129	THR
3	N	1184	GLN
3	N	1267	ARG
3	N	1307	LYS
4	O	49	GLN
5	P	95	THR
5	P	295	MET
5	P	323	ASP
5	P	325	LYS
5	P	380	GLU
5	P	396	ARG
5	P	417	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	213	GLN
2	C	99	GLN
2	C	102	HIS
2	C	390	GLN
2	C	434	HIS
2	C	538	GLN
2	C	899	GLN
2	C	1026	GLN
3	D	66	GLN
3	D	560	GLN
3	D	669	ASN
3	D	724	GLN
3	D	976	GLN
3	D	1046	GLN
3	D	1172	HIS
3	D	1184	GLN
3	D	1195	GLN
5	F	83	GLN
5	F	411	HIS
2	M	219	GLN
3	N	66	GLN
3	N	724	GLN
3	N	994	GLN
3	N	1184	GLN
3	N	1254	GLN
3	N	1359	GLN
3	N	1374	GLN
4	O	33	HIS
4	O	49	GLN
5	P	83	GLN
5	P	402	ASN

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 13 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
12	COD	D	2008	10	25,30,46	1.73	7 (28%)	28,46,68	1.80	6 (21%)
11	DPO	D	2006	8	6,8,8	0.96	0	13,13,13	1.16	1 (7%)
11	DPO	N	1606	8	6,8,8	0.98	0	13,13,13	1.07	1 (7%)
12	COD	N	1608	10	24,29,46	1.77	5 (20%)	29,45,68	1.68	6 (20%)

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
12	COD	D	2008	10	-	3/15/35/59	0/3/3/3
11	DPO	D	2006	8	-	0/6/6/6	-
11	DPO	N	1606	8	-	0/6/6/6	-
12	COD	N	1608	10	-	6/12/32/59	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	2008	COD	C2-N3	4.67	1.39	1.32
12	N	1608	COD	C2-N3	4.53	1.39	1.32
12	N	1608	COD	C18-C16	3.09	1.61	1.51
12	D	2008	COD	C18-C16	3.04	1.61	1.51
12	N	1608	COD	C2-N1	2.70	1.38	1.33
12	N	1608	COD	C6-N7	2.68	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	2008	COD	C6-N7	2.67	1.43	1.34
12	D	2008	COD	C2-N1	2.66	1.38	1.33
12	N	1608	COD	O13-C12	-2.38	1.37	1.43
12	D	2008	COD	O13-C12	-2.34	1.37	1.43
12	D	2008	COD	O15-C14	-2.01	1.38	1.43
12	D	2008	COD	C6-C5	-2.01	1.35	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	N	1608	COD	N3-C2-N1	-5.19	120.57	128.68
12	D	2008	COD	N3-C2-N1	-5.16	120.61	128.68
12	D	2008	COD	C14-C12-C11	4.58	107.87	100.98
12	N	1608	COD	C14-C12-C11	3.74	106.61	100.98
12	N	1608	COD	P20-O23-P24	-3.68	120.20	132.83
12	D	2008	COD	P24-O23-P20	-3.19	121.87	132.83
12	D	2008	COD	O23-P24-O27	2.89	111.59	102.58
11	D	2006	DPO	P2-O4-P1	-2.79	123.25	132.83
11	N	1606	DPO	P2-O4-P1	-2.76	123.34	132.83
12	N	1608	COD	C4-C5-N8	2.44	111.94	109.40
12	D	2008	COD	C4-C5-N8	2.42	111.92	109.40
12	D	2008	COD	O17-C16-C18	2.17	116.52	109.37
12	N	1608	COD	C2-N1-C6	2.09	122.34	118.75
12	N	1608	COD	O17-C16-C18	2.03	116.05	109.37

There are no chirality outliers.

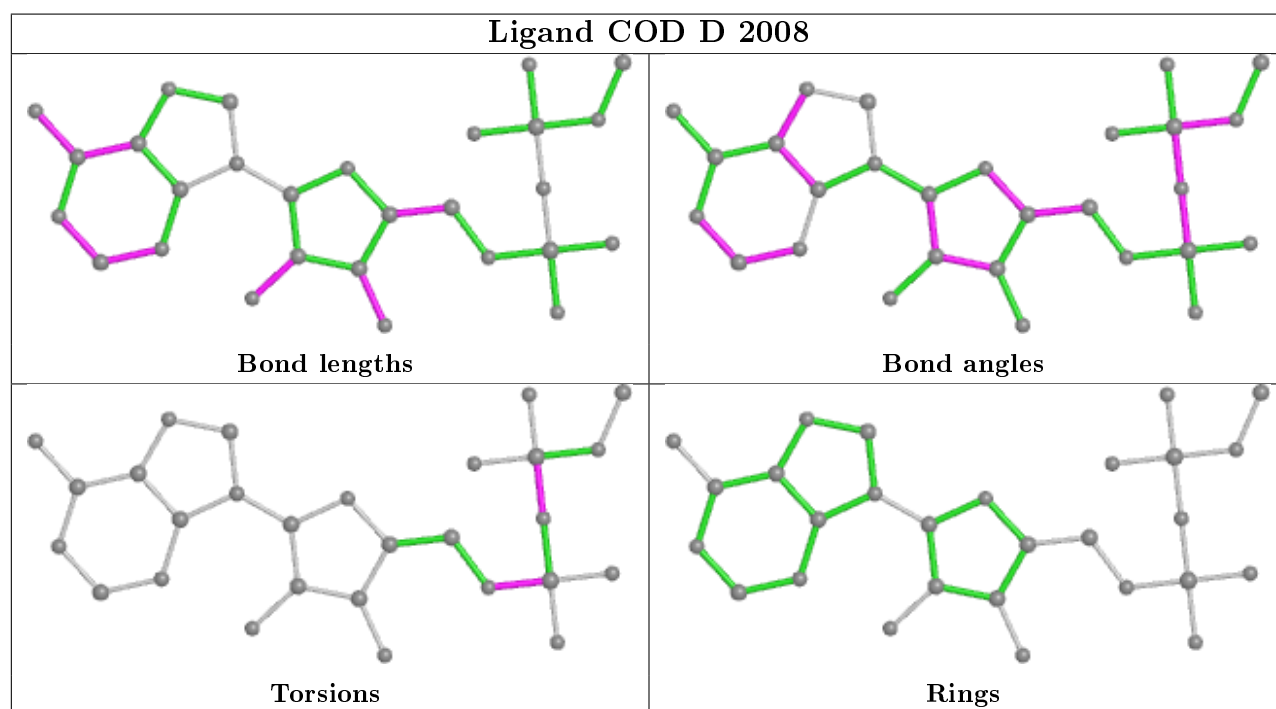
All (9) torsion outliers are listed below:

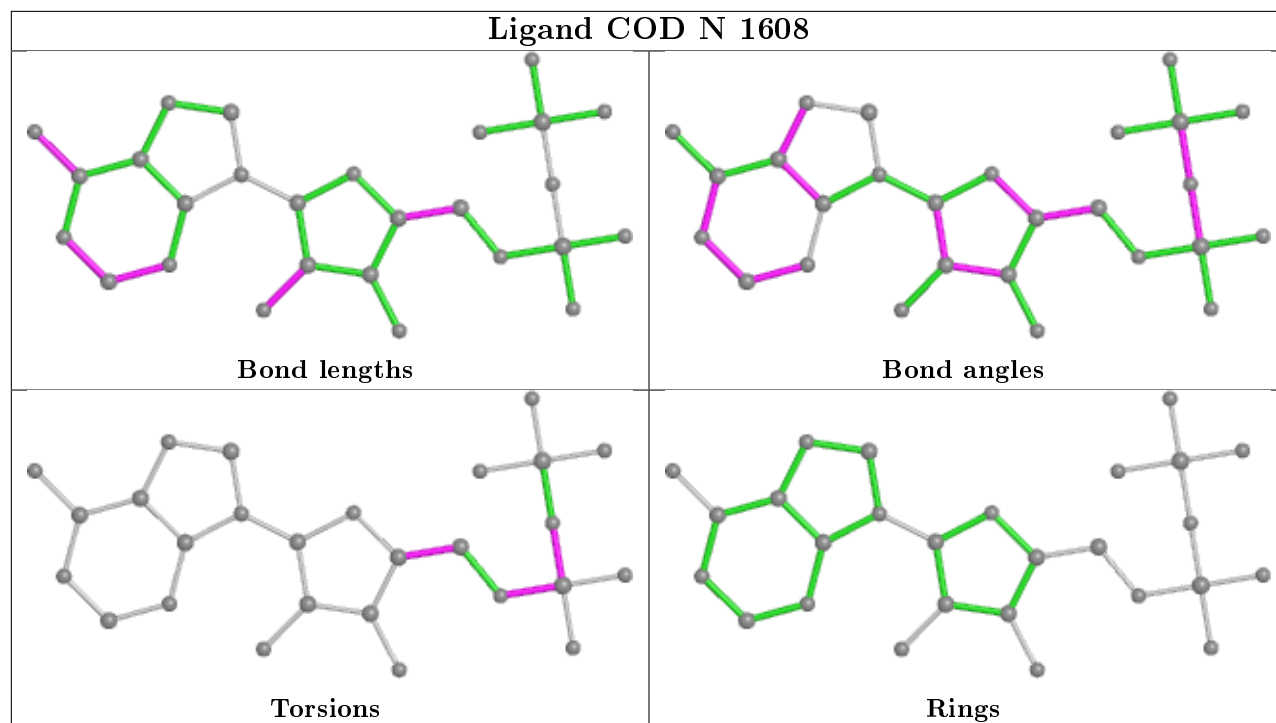
Mol	Chain	Res	Type	Atoms
12	N	1608	COD	C18-O19-P20-O21
12	N	1608	COD	C18-O19-P20-O22
12	N	1608	COD	C18-O19-P20-O23
12	N	1608	COD	O17-C16-C18-O19
12	N	1608	COD	C14-C16-C18-O19
12	D	2008	COD	P20-O23-P24-O27
12	N	1608	COD	P24-O23-P20-O22
12	D	2008	COD	P20-O23-P24-O26
12	D	2008	COD	C18-O19-P20-O22

There are no ring outliers.

No monomer is involved in short contacts.

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	231/315 (73%)	-0.17	5 (2%) 62 39	29, 51, 78, 126	1 (0%)
1	B	223/315 (70%)	-0.28	2 (0%) 84 68	26, 53, 93, 122	0
1	K	231/315 (73%)	-0.39	5 (2%) 62 39	22, 38, 65, 128	1 (0%)
1	L	223/315 (70%)	-0.33	0 100 100	21, 49, 82, 102	0
2	C	1112/1119 (99%)	0.07	49 (4%) 34 17	12, 58, 115, 132	3 (0%)
2	M	1112/1119 (99%)	-0.35	11 (0%) 82 66	5, 32, 82, 118	3 (0%)
3	D	1486/1524 (97%)	-0.17	22 (1%) 73 53	7, 43, 96, 131	4 (0%)
3	N	1486/1524 (97%)	-0.29	11 (0%) 87 74	4, 34, 85, 125	4 (0%)
4	E	94/99 (94%)	-0.24	2 (2%) 63 41	22, 44, 88, 102	0
4	O	94/99 (94%)	-0.44	1 (1%) 80 63	14, 31, 67, 85	0
5	F	346/443 (78%)	0.26	27 (7%) 13 4	33, 70, 134, 152	0
5	P	346/443 (78%)	-0.20	5 (1%) 75 55	14, 43, 93, 112	0
6	H	21/27 (77%)	0.56	3 (14%) 2 1	47, 92, 134, 155	0
6	S	21/27 (77%)	0.30	3 (14%) 2 1	35, 73, 118, 146	0
7	G	16/19 (84%)	0.55	1 (6%) 20 8	49, 77, 129, 134	0
7	R	16/19 (84%)	0.54	2 (12%) 3 1	31, 60, 131, 137	0
All	All	7058/7722 (91%)	-0.18	149 (2%) 63 41	4, 45, 99, 155	16 (0%)

All (149) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	63	GLY	9.3
5	F	391	GLY	7.3
1	A	233	VAL	7.2
5	F	390	PHE	5.8
1	K	233	VAL	5.8

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Mol	Chain	Res	Type	RSRZ
2	M	365	ASP	5.7
1	A	234	ALA	5.3
1	K	232	ALA	5.3
1	K	234	ALA	5.2
1	A	232	ALA	5.1
5	F	377	ASP	4.9
5	F	389	PHE	4.8
5	F	381	HIS	4.8
2	C	362	GLY	4.7
2	C	200	LEU	4.4
2	C	188	LYS	4.4
2	C	363	SER	4.4
3	D	191	LEU	4.0
2	C	809	GLY	3.9
5	F	410	TYR	3.9
3	N	1252	ILE	3.8
5	F	392	VAL	3.7
3	D	70	GLY	3.7
7	G	19	DA	3.6
2	M	219	GLN	3.6
2	C	769	PRO	3.6
6	H	25	DA	3.5
5	F	411	HIS	3.5
6	S	25	DA	3.5
2	C	86	LYS	3.5
2	C	107	LEU	3.5
3	N	1499	ARG	3.5
5	F	414	ARG	3.5
6	H	24	DC	3.5
3	D	194	GLY	3.4
2	M	104	ASP	3.3
2	C	104	ASP	3.3
5	F	326	ASP	3.3
3	D	423	ASP	3.2
3	N	1297	GLU	3.2
2	M	766	GLU	3.2
2	C	251	ASP	3.2
5	F	356	LYS	3.1
3	D	372	ASP	3.1
5	F	325	LYS	3.1
3	N	991	GLN	3.1
2	C	770	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
2	C	65	VAL	3.1
3	D	373	PRO	3.0
2	C	367	LEU	3.0
5	F	359	SER	3.0
5	F	386	VAL	2.9
2	C	294	GLU	2.9
3	D	405	ASP	2.9
2	C	649	VAL	2.8
5	F	415	THR	2.8
7	R	19	DA	2.8
2	C	105	THR	2.8
2	C	48	PHE	2.8
2	C	421	GLU	2.8
2	C	109	LYS	2.8
5	P	382	THR	2.8
3	N	173	PRO	2.8
5	F	142	ARG	2.7
2	M	364	GLU	2.7
3	D	1127	GLU	2.7
2	C	295	ASP	2.7
6	S	24	DC	2.7
3	D	1495	ILE	2.7
3	D	1499	ARG	2.7
3	N	144	GLY	2.7
2	C	68	PHE	2.6
2	C	296	GLY	2.6
5	F	376	ILE	2.6
1	A	231	ALA	2.6
5	F	138	SER	2.6
5	F	393	THR	2.6
3	D	235	ALA	2.5
2	C	196	LEU	2.5
2	C	365	ASP	2.5
2	C	622	GLU	2.5
5	P	324	GLU	2.5
6	H	23	DG	2.5
6	S	23	DG	2.5
2	C	597	ALA	2.5
3	D	195	VAL	2.4
2	C	258	TYR	2.4
2	C	52	PHE	2.4
3	N	976	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
3	D	198	ARG	2.4
2	C	106	GLY	2.4
2	C	292	ARG	2.4
2	C	255	ALA	2.4
2	C	358	ARG	2.4
2	M	650	ARG	2.3
3	D	318	ARG	2.3
2	C	242	LEU	2.3
3	D	378	ILE	2.3
2	C	246	ASP	2.3
2	M	366	SER	2.3
4	O	51	LEU	2.3
5	F	147	LEU	2.3
2	C	66	LEU	2.3
5	F	139	ALA	2.3
3	D	209	ARG	2.3
2	C	108	ILE	2.3
2	C	300	ASP	2.3
7	R	4	DT	2.3
2	C	361	MET	2.3
2	M	362	GLY	2.2
5	P	149	GLU	2.2
3	D	68	PHE	2.2
1	K	231	ALA	2.2
2	C	766	GLU	2.2
3	N	805	GLU	2.2
1	B	134	GLU	2.2
2	C	286	SER	2.2
3	N	982	PHE	2.2
2	C	739	GLU	2.2
2	C	221	LEU	2.2
2	C	102	HIS	2.2
2	M	63	GLY	2.2
5	F	146	GLY	2.2
1	A	230	ALA	2.2
2	M	811	PRO	2.2
3	D	190	GLU	2.2
2	C	1105	LYS	2.1
5	P	423	ASP	2.1
2	C	777	ILE	2.1
3	D	805	GLU	2.1
3	N	977	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
5	P	325	LYS	2.1
3	D	406	ASP	2.1
4	E	83	ASP	2.1
5	F	395	GLU	2.1
1	B	186	LEU	2.1
3	N	219	GLU	2.1
4	E	84	ARG	2.1
1	K	19	GLU	2.1
2	M	421	GLU	2.1
2	C	240	THR	2.1
2	C	226	VAL	2.1
5	F	301	ALA	2.1
5	F	407	LYS	2.0
3	D	307	ALA	2.0
3	D	237	LYS	2.0
5	F	121	GLY	2.0
2	C	2	GLU	2.0
5	F	408	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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	MG	B	2001	1/1	0.74	0.29	71,71,71,71	0
12	COD	D	2008	28/44	0.77	0.40	50,73,102,116	28
8	MG	F	2001	1/1	0.81	0.18	92,92,92,92	0
8	MG	P	2001	1/1	0.87	0.13	38,38,38,38	0
10	C	D	2005	20/21	0.88	0.25	43,61,71,80	20

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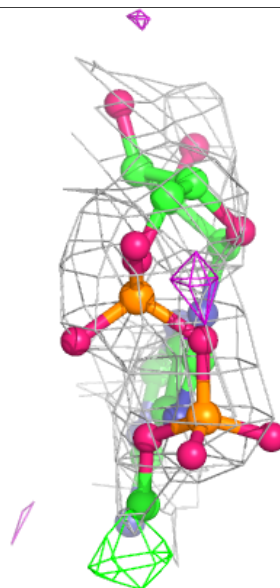
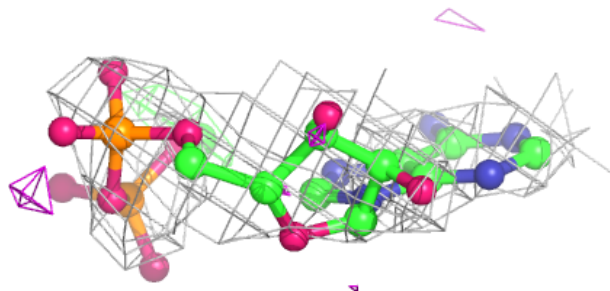
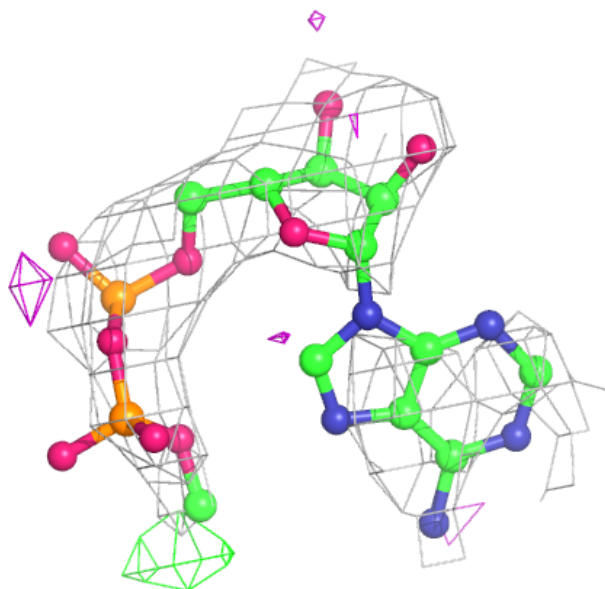
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
12	COD	N	1608	27/44	0.89	0.23	35,43,62,65	27
10	C	N	1605	20/21	0.90	0.20	24,34,49,57	20
11	DPO	N	1606	9/9	0.90	0.19	26,51,74,84	0
8	MG	D	2007	1/1	0.92	0.17	49,49,49,49	0
11	DPO	D	2006	9/9	0.93	0.21	45,68,84,98	0
8	MG	N	1607	1/1	0.95	0.17	36,36,36,36	0
8	MG	D	2003	1/1	0.96	0.15	22,22,22,22	0
8	MG	N	1601	1/1	0.97	0.44	25,25,25,25	0
9	ZN	D	2002	1/1	0.97	0.04	92,92,92,92	0
8	MG	D	2004	1/1	0.97	0.43	27,27,27,27	0
9	ZN	N	1602	1/1	0.99	0.13	16,16,16,16	0
8	MG	N	1604	1/1	0.99	0.19	13,13,13,13	0
9	ZN	N	1603	1/1	0.99	0.05	50,50,50,50	0
9	ZN	D	2001	1/1	1.00	0.13	20,20,20,20	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.

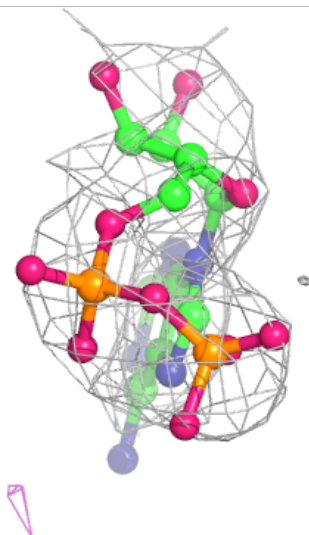
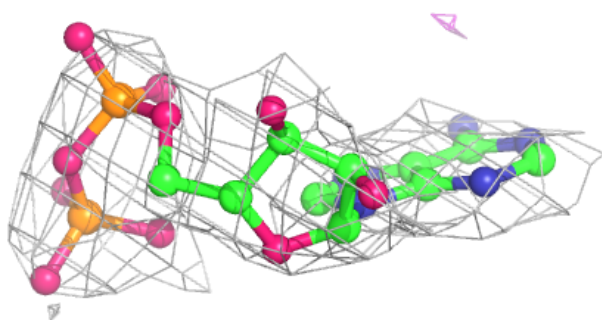
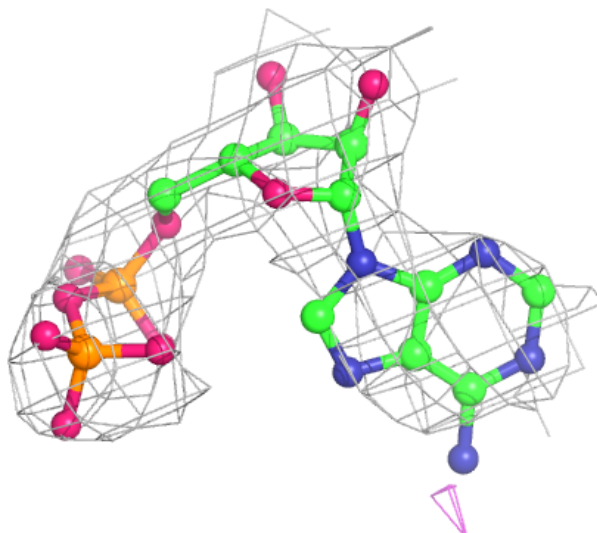
Electron density around COD D 2008:

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



Electron density around COD N 1608:

$2mF_o-DF_c$ (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.