



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:26 PM UTC

PDB ID : 5D4D / pdb_00005d4d
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

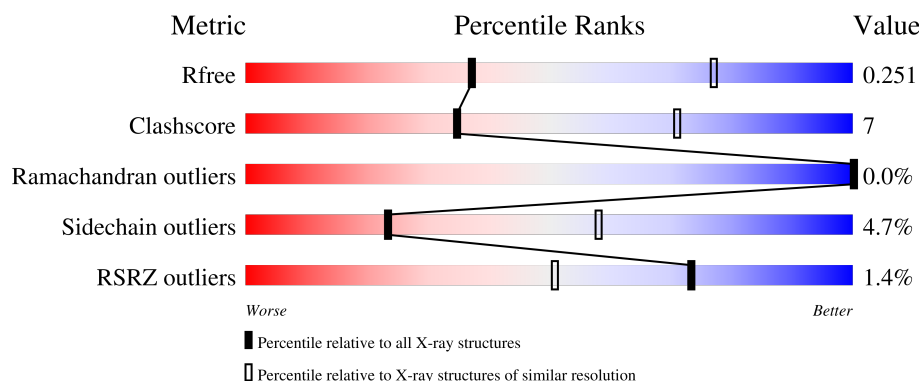
1 Overall quality at a glance

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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 of 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	
1	B	315	
1	K	315	
1	L	315	
2	C	1119	

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Mol	Chain	Length	Quality of chain
2	M	1119	
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 15 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			

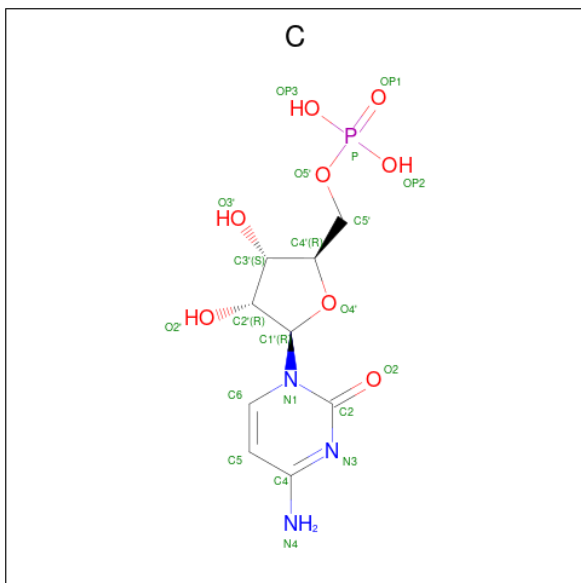
- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

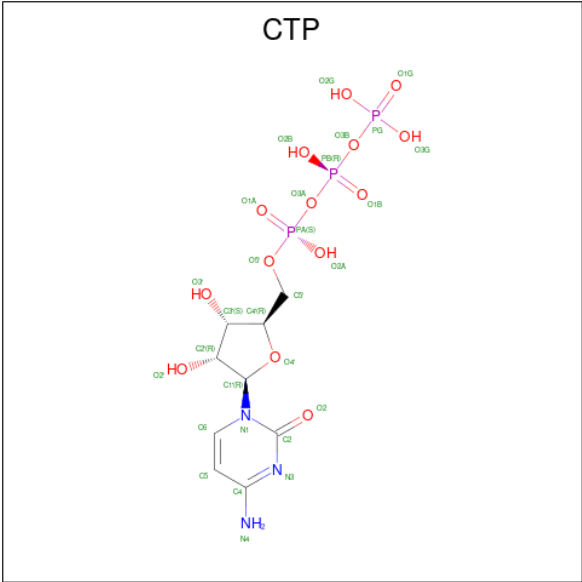
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	D	2	Total	Zn	0	0
			2	2		
9	N	2	Total	Zn	0	0
			2	2		

- Molecule 10 is CYTIDINE-5'-MONOPHOSPHATE (CCD ID: C) (formula: C₉H₁₄N₃O₈P).



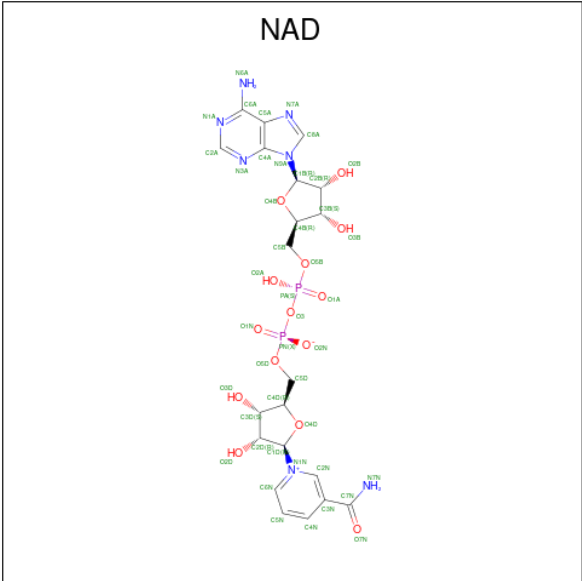
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	D	1	Total	C	N	O	P	0	0
			20	9	3	7	1		

- Molecule 11 is CYTIDINE-5'-TRIPHOSPHATE (CCD ID: CTP) (formula: C₉H₁₆N₃O₁₄P₃).



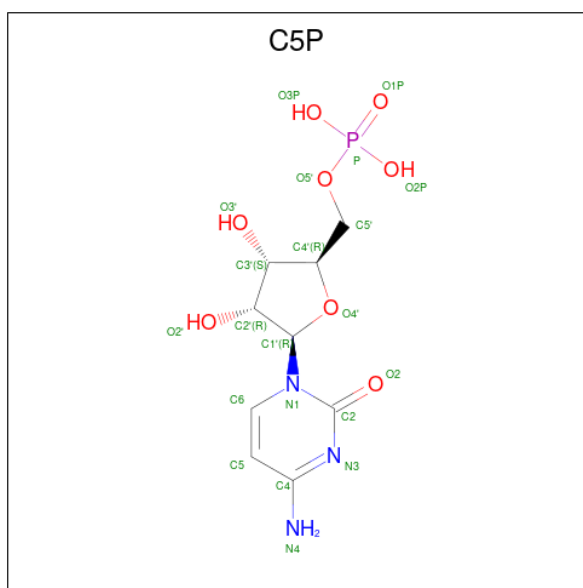
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	D	1	Total	O	P		0	0
			9	7	2			
11	M	1	Total	O	P		0	0
			9	7	2			

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



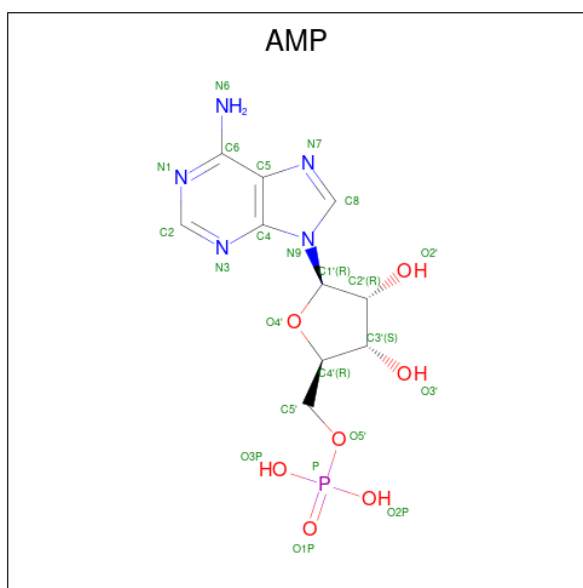
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 13 is CYTIDINE-5'-MONOPHOSPHATE (CCD ID: C5P) (formula: $C_9H_{14}N_3O_8P$).



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

- Molecule 14 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



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

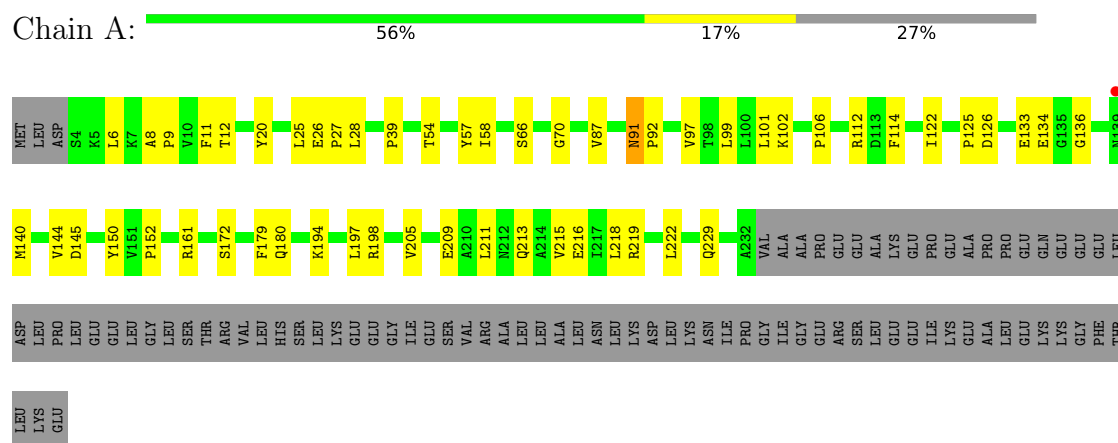
- Molecule 15 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	23	Total O 23 23	0	0
15	B	16	Total O 16 16	0	0
15	C	196	Total O 196 196	0	0
15	D	243	Total O 243 243	0	0
15	E	16	Total O 16 16	0	0
15	F	45	Total O 45 45	0	0
15	G	9	Total O 9 9	0	0
15	H	4	Total O 4 4	0	0
15	K	14	Total O 14 14	0	0
15	L	13	Total O 13 13	0	0
15	M	97	Total O 97 97	0	0
15	N	187	Total O 187 187	0	0
15	O	12	Total O 12 12	0	0
15	P	14	Total O 14 14	0	0
15	R	3	Total O 3 3	0	0
15	S	3	Total O 3 3	0	0

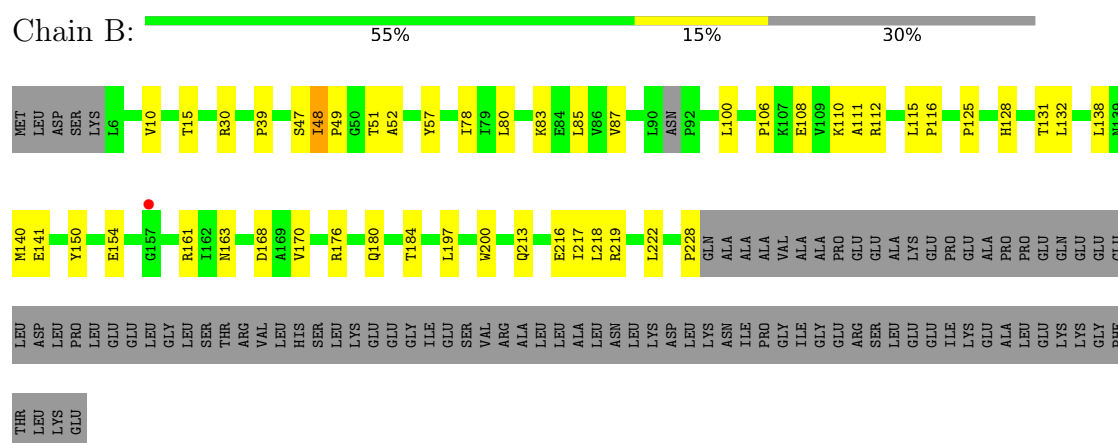
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

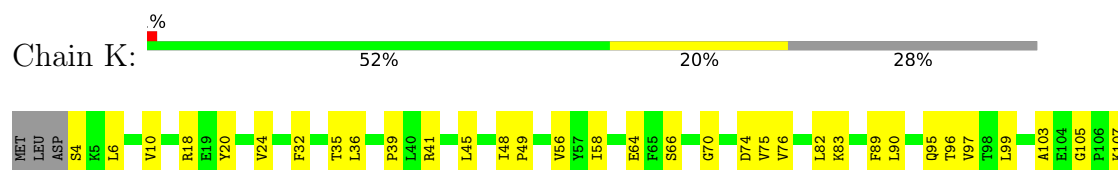
- Molecule 1: DNA-directed RNA polymerase subunit alpha

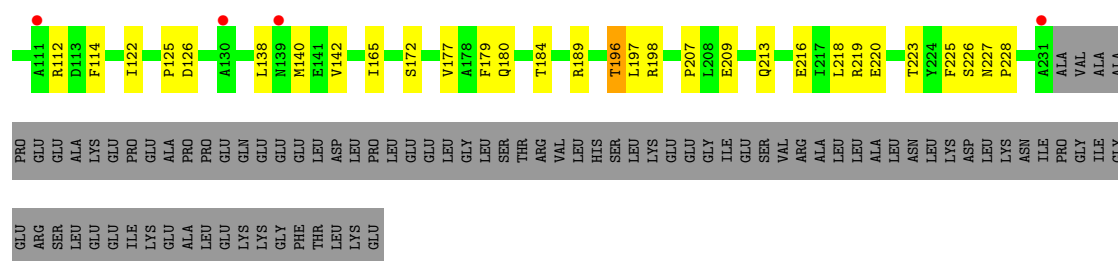


- Molecule 1: DNA-directed RNA polymerase subunit alpha

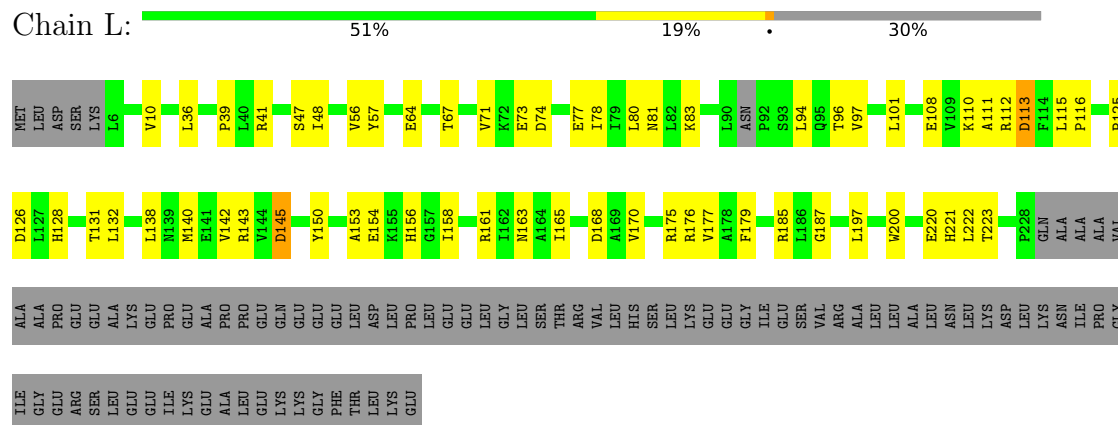


- Molecule 1: DNA-directed RNA polymerase subunit alpha

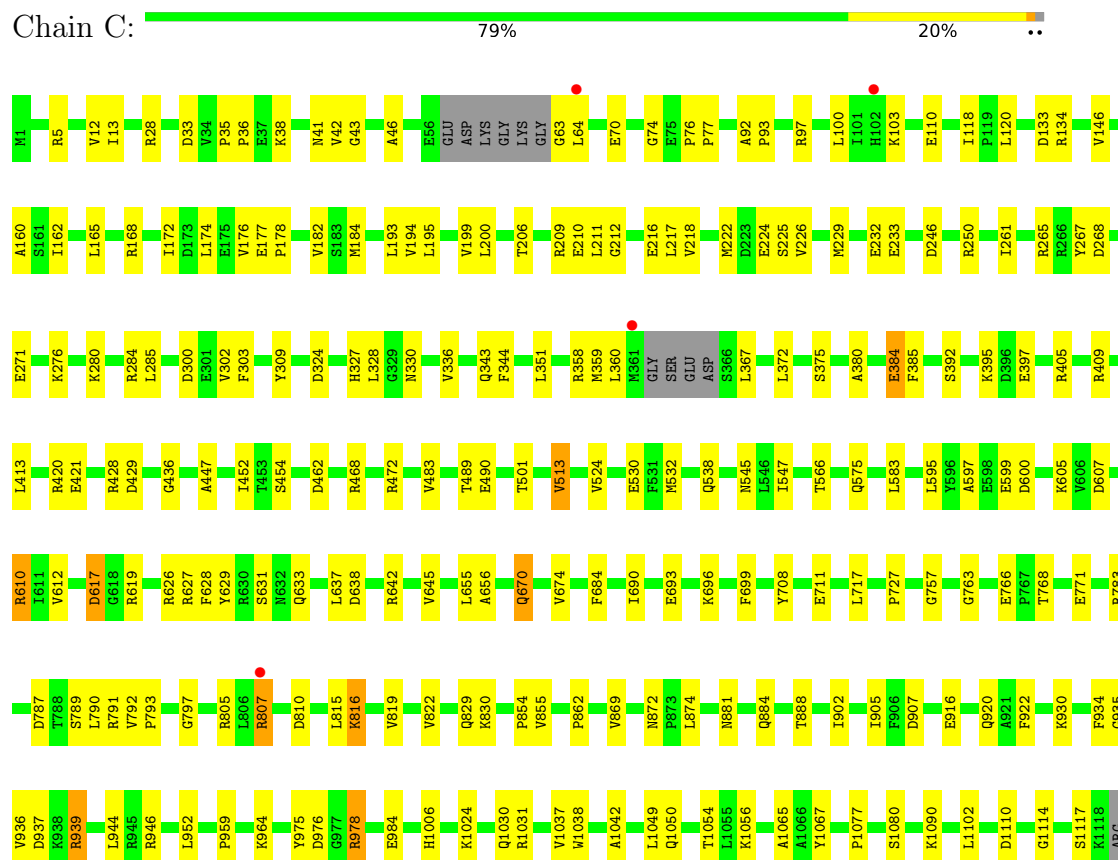




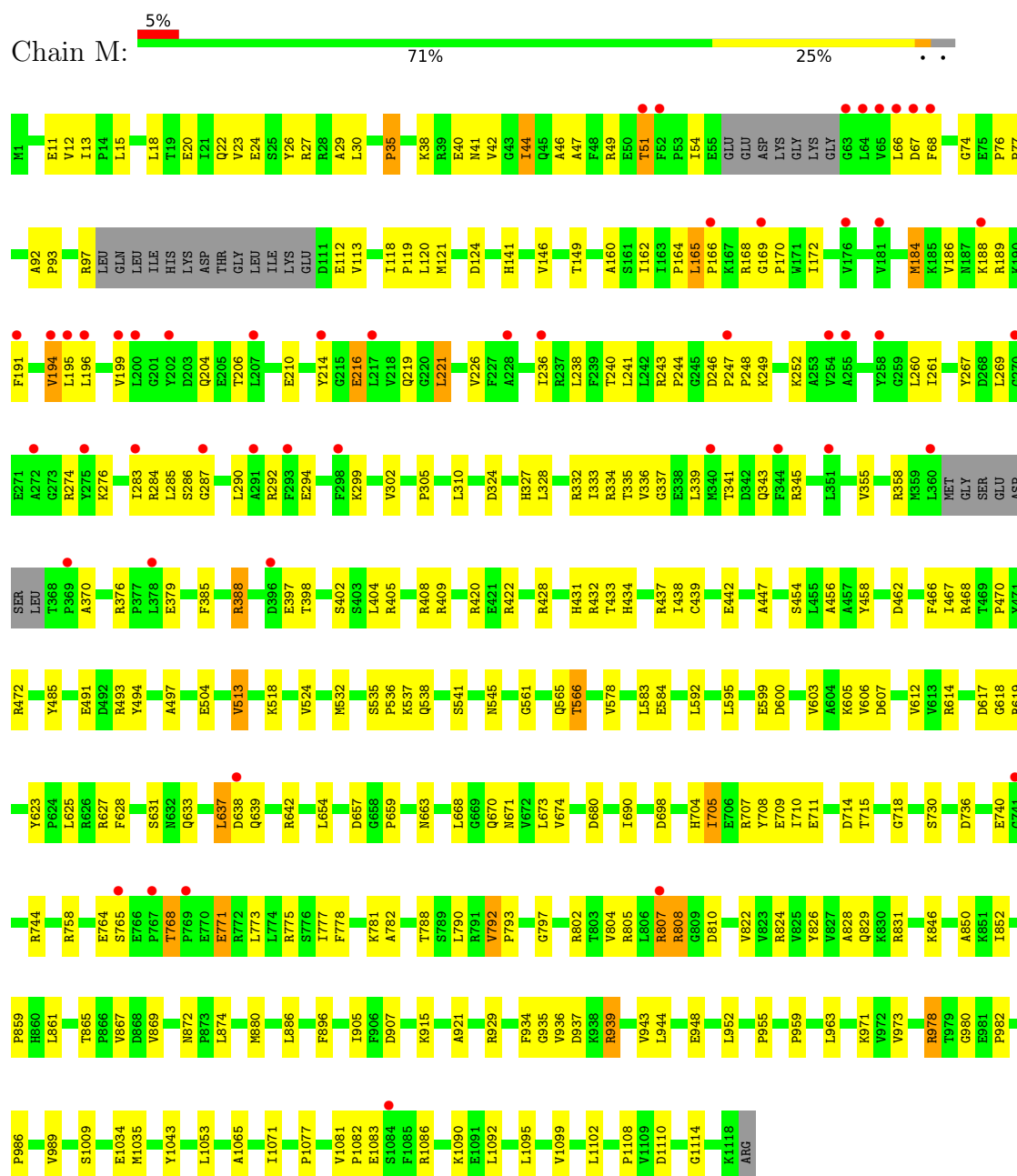
• Molecule 1: DNA-directed RNA polymerase subunit alpha



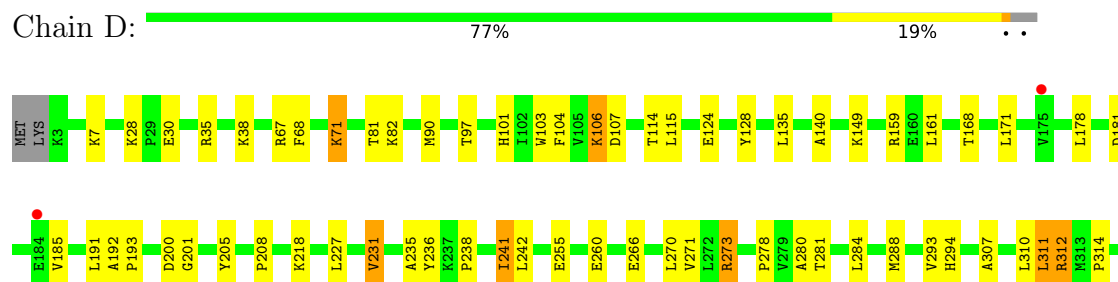
• Molecule 2: DNA-directed RNA polymerase subunit beta

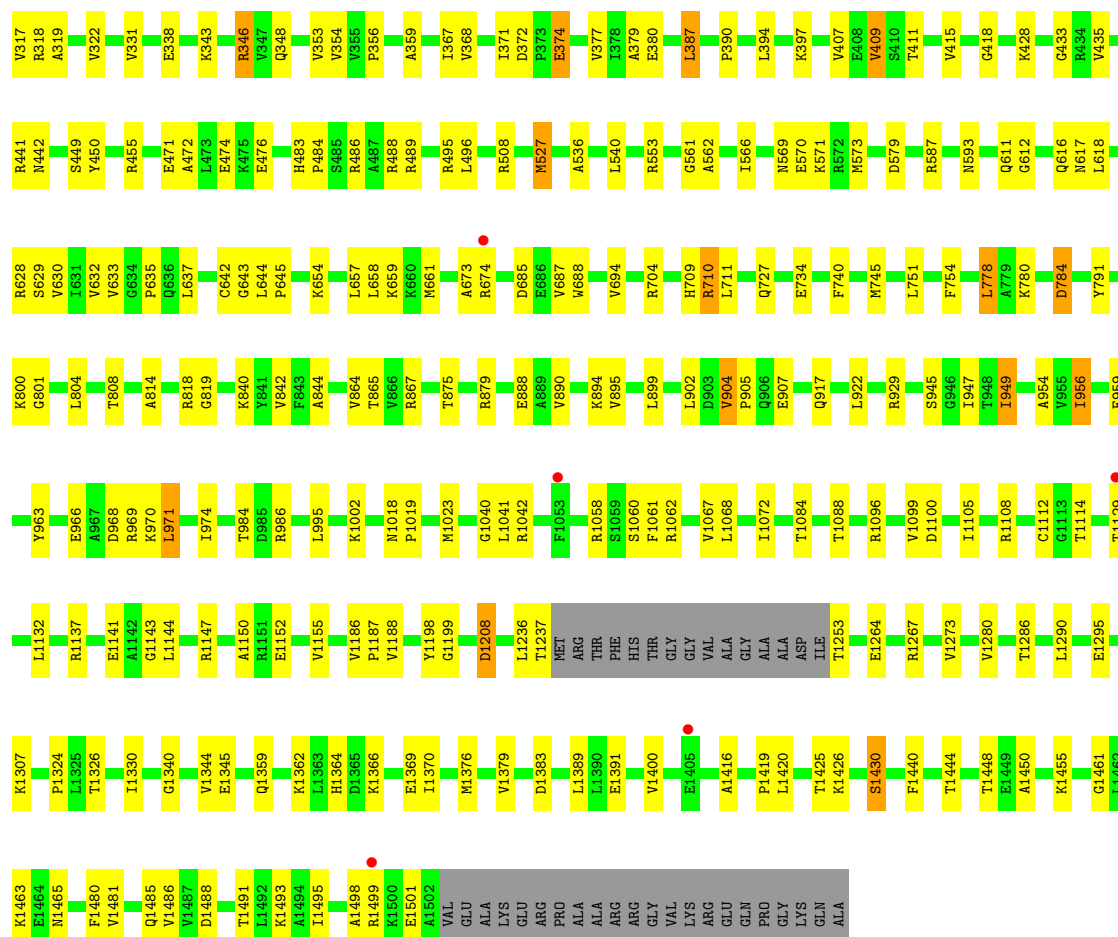


• Molecule 2: DNA-directed RNA polymerase subunit beta

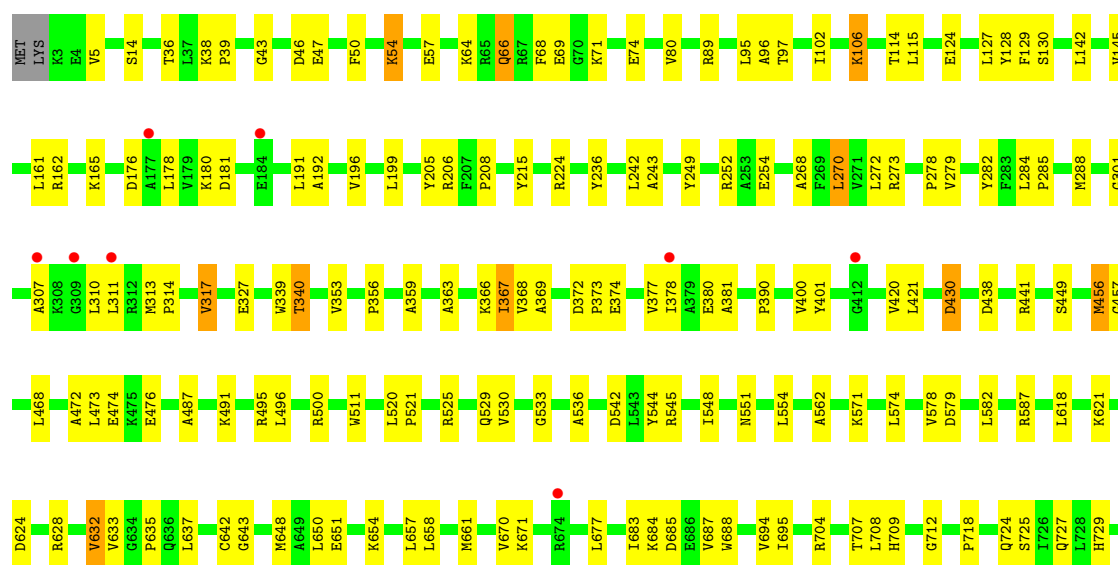
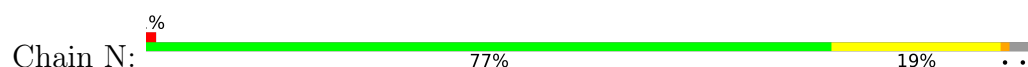


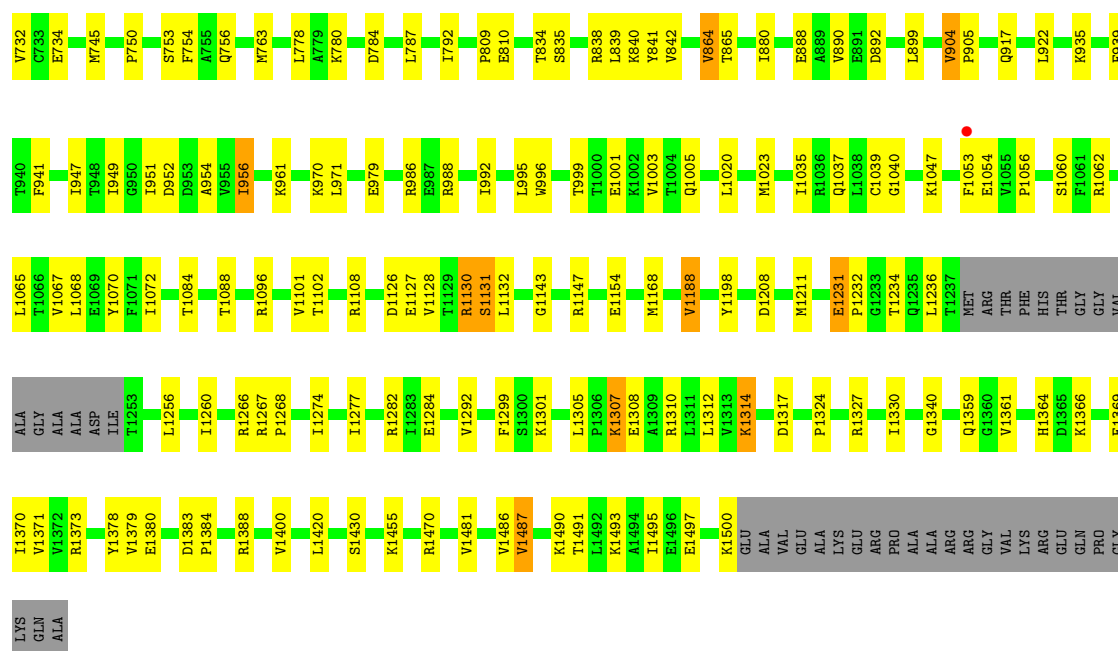
• Molecule 3: DNA-directed RNA polymerase subunit beta'





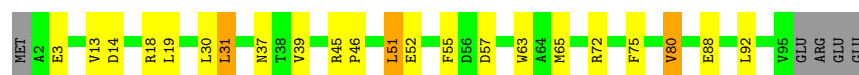
• Molecule 3: DNA-directed RNA polymerase subunit beta'





- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E: 73% 19% 5%



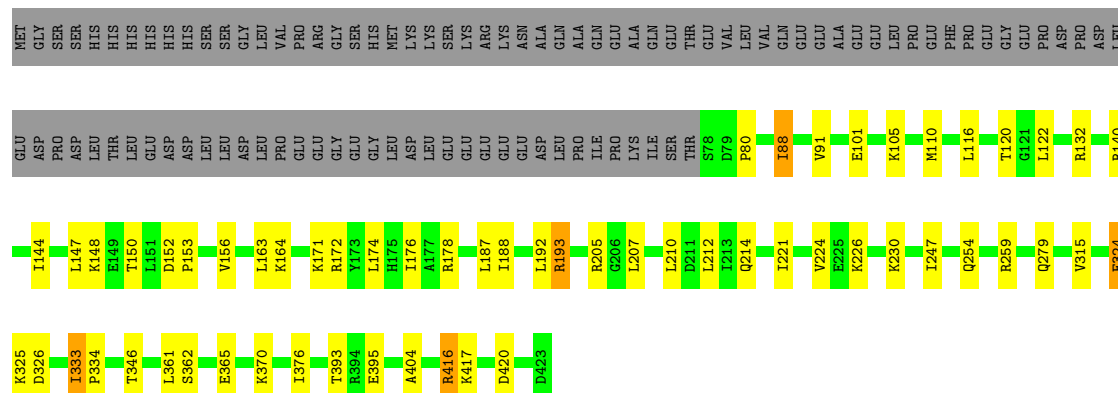
- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain O: 81% 12% 5%

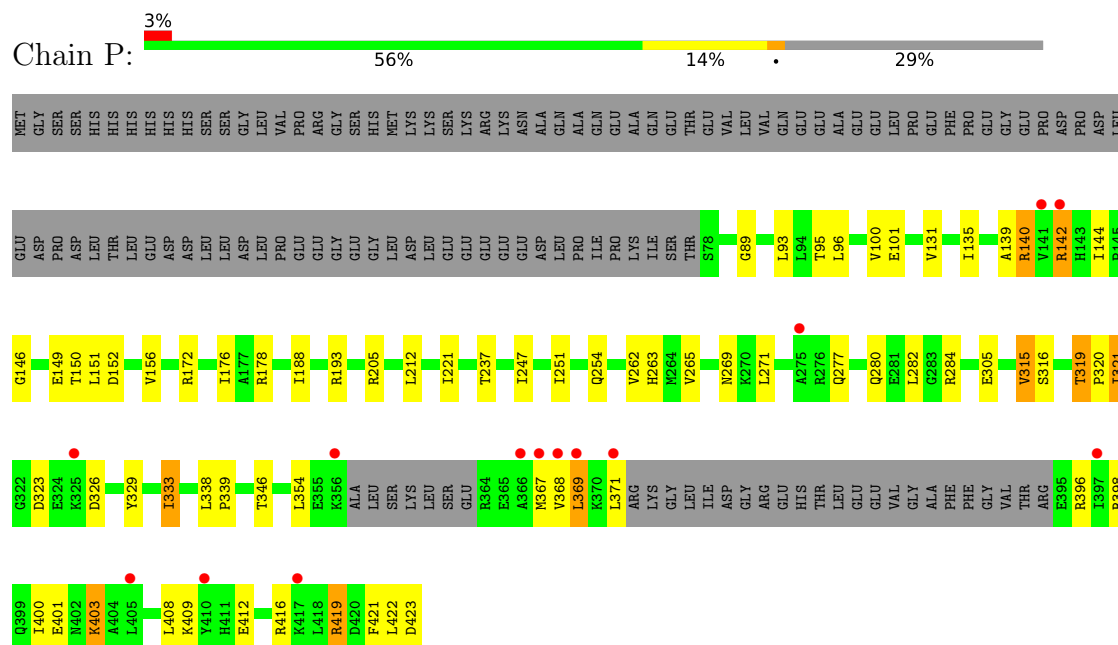


- Molecule 5: RNA polymerase sigma factor SigA

Chain F: 65% 12% 22%



- Molecule 5: RNA polymerase sigma factor SigA



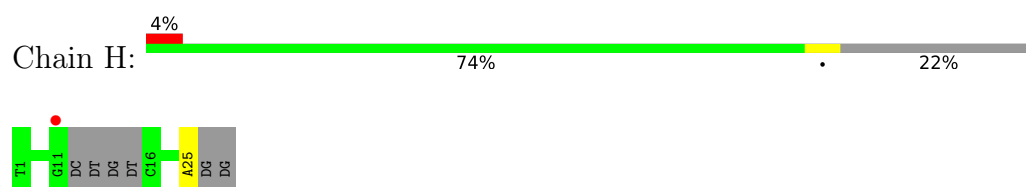
- Molecule 6: DNA (5'-D(*CP*C*TP*GP*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*TP*AP*GP*AP*G)-3')



- 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')

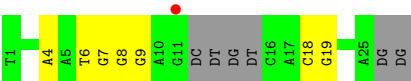


- Molecule 7: DNA (27-MER)



- 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, α , β , γ	185.00Å 103.51Å 296.30Å 90.00° 98.27° 90.00°	Depositor
Resolution (Å)	42.17 – 3.00 42.17 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.5 (42.17-3.00) 97.9 (42.17-3.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.8-1069	Depositor
R, R_{free}	0.201 , 0.254 0.202 , 0.251	Depositor DCC
R_{free} test set	10942 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	48.8	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 29.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	57349	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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: C5P, CTP, MG, AMP, NAD, ZN

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	0.38	0/1829	0.89	6/2487 (0.2%)
1	B	0.36	0/1781	0.84	3/2420 (0.1%)
1	K	0.35	0/1824	0.80	3/2480 (0.1%)
1	L	0.35	0/1781	0.85	3/2420 (0.1%)
2	C	0.41	0/8913	0.83	5/12053 (0.0%)
2	M	0.38	0/8775	0.83	9/11867 (0.1%)
3	D	0.41	0/11936	0.81	10/16138 (0.1%)
3	N	0.39	0/11922	0.81	6/16119 (0.0%)
4	E	0.38	0/772	0.82	0/1040
4	O	0.34	0/772	0.79	0/1040
5	F	0.38	0/2852	0.81	2/3837 (0.1%)
5	P	0.36	0/2614	0.84	4/3516 (0.1%)
6	G	0.37	1/368 (0.3%)	0.61	0/567
6	R	0.17	0/368	0.63	0/567
7	H	0.21	0/489	0.72	0/752
7	S	0.18	0/488	0.67	0/750
All	All	0.39	1/57484 (0.0%)	0.82	51/78053 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	18	DG	O3'-P	-5.66	1.52	1.61

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	1340	GLY	CA-C-N	7.50	126.77	118.97
3	N	1340	GLY	C-N-CA	7.50	126.77	118.97
3	D	1208	ASP	N-CA-C	-7.40	97.20	108.67
2	C	271	GLU	N-CA-C	-7.32	103.33	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	P	326	ASP	N-CA-C	6.98	118.97	111.36
3	N	1231	GLU	CA-C-N	-6.85	111.27	119.84
3	N	1231	GLU	C-N-CA	-6.85	111.27	119.84
5	F	417	LYS	N-CA-C	6.61	118.48	111.28
3	D	1340	GLY	CA-C-N	6.54	125.77	118.97
3	D	1340	GLY	C-N-CA	6.54	125.77	118.97
2	C	336	VAL	CB-CA-C	-6.46	103.61	111.88
2	C	303	PHE	N-CA-C	6.39	118.78	111.11
3	D	1186	VAL	N-CA-C	6.27	114.88	107.73
1	L	47	SER	N-CA-C	6.22	121.00	113.17
1	B	47	SER	N-CA-C	6.19	120.97	113.17
2	M	792	VAL	CA-C-N	6.06	124.02	119.66
2	M	792	VAL	C-N-CA	6.06	124.02	119.66
2	M	765	SER	CB-CA-C	-5.89	108.78	115.79
1	A	8	ALA	CA-C-N	5.78	126.26	120.14
1	A	8	ALA	C-N-CA	5.78	126.26	120.14
1	A	91	ASN	CA-C-N	5.75	125.42	119.56
1	A	91	ASN	C-N-CA	5.75	125.42	119.56
3	D	617	ASN	N-CA-C	5.67	120.32	113.17
3	N	1481	VAL	N-CA-C	5.65	118.42	112.83
1	A	172	SER	CA-C-N	5.60	125.22	119.56
1	A	172	SER	C-N-CA	5.60	125.22	119.56
5	P	262	VAL	N-CA-C	5.57	116.97	110.62
3	D	1481	VAL	N-CA-C	5.55	118.33	112.83
5	F	333	ILE	N-CA-C	5.54	113.03	107.55
3	N	1208	ASP	N-CA-C	-5.53	100.79	109.25
2	C	302	VAL	N-CA-C	5.51	116.58	111.45
2	C	547	ILE	N-CA-C	5.49	112.56	107.56
1	L	48	ILE	CA-C-N	5.49	125.76	119.83
1	L	48	ILE	C-N-CA	5.49	125.76	119.83
3	D	1286	THR	N-CA-C	-5.46	102.40	110.48
2	M	388	ARG	N-CA-C	5.38	119.95	113.17
5	P	139	ALA	N-CA-C	-5.34	99.42	110.80
3	D	28	LYS	CA-C-N	5.34	125.42	119.87
3	D	28	LYS	C-N-CA	5.34	125.42	119.87
1	K	172	SER	CA-C-N	5.32	124.93	119.56
1	K	172	SER	C-N-CA	5.32	124.93	119.56
2	M	35	PRO	CA-C-N	5.28	125.59	119.47
2	M	35	PRO	C-N-CA	5.28	125.59	119.47
1	K	165	ILE	CB-CA-C	-5.21	105.19	111.18
3	D	740	PHE	N-CA-C	5.18	118.63	112.72
2	M	980	GLY	N-CA-C	-5.11	107.48	114.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	P	333	ILE	N-CA-C	5.06	113.50	107.73
1	B	48	ILE	CA-C-N	5.04	125.27	119.83
1	B	48	ILE	C-N-CA	5.04	125.27	119.83
2	M	439	CYS	CA-C-N	5.01	124.62	119.56
2	M	439	CYS	C-N-CA	5.01	124.62	119.56

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	41	0
1	L	1750	0	1802	43	0
2	C	8747	0	8858	124	0
2	M	8611	0	8710	176	0
3	D	11730	0	11960	168	0
3	N	11716	0	11949	180	1
4	E	758	0	770	14	0
4	O	758	0	770	9	0
5	F	2807	0	2882	42	0
5	P	2574	0	2643	45	1
6	G	328	0	182	7	0
6	R	328	0	182	4	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	D	20	0	11	0	0
11	D	9	0	0	0	0
11	M	9	0	0	0	0
12	G	44	0	24	1	0
13	N	20	0	11	3	0
14	R	23	0	11	0	0
15	A	23	0	0	0	0
15	B	16	0	0	0	0
15	C	196	0	0	2	0
15	D	243	0	0	7	0
15	E	16	0	0	0	0
15	F	45	0	0	1	0
15	G	9	0	0	0	0
15	H	4	0	0	0	0
15	K	14	0	0	0	0
15	L	13	0	0	1	0
15	M	97	0	0	5	0
15	N	187	0	0	2	0
15	O	12	0	0	0	0
15	P	14	0	0	1	0
15	R	3	0	0	0	0
15	S	3	0	0	0	0
All	All	57349	0	56733	840	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 (840) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1108:ARG:NH2	3:D:1198:TYR:O	2.21	0.72
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
3:D:949:ILE:HD11	3:D:1023:MET:HE1	1.71	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
3:N:657:LEU:HG	3:N:661:MET:HE2	1.75	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
2:M:846:LYS:NZ	13:N:2005:C5P:O1P	2.22	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	15: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
2:C:501:THR:HB	2:C:532:MET:HE3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:343:GLN:HG3	2:C:385:PHE:HB2	1.79	0.64
2:C:172:ILE:HD13	2:C:184:MET:HE3	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:273:ARG:HB3	3:N:278:PRO:HA	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1040:GLY:O	3:N:1060:SER:HB3	2.00	0.60
3:D:343:LYS:NZ	3:D:380:GLU:OE1	2.29	0.60
4:E:3:GLU:HB3	4:E:65:MET:HE1	1.83	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
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
3:D:284:LEU:HD22	3:D:288:MET:HE2	1.83	0.60
2:C:816:LYS:HG3	2:C:819:VAL:HG21	1.82	0.60
3:D:566:ILE:HD11	5:F:192:LEU:HD21	1.83	0.60
2:M:1092:LEU:HD13	2:M:1099:VAL:HG21	1.84	0.60
2:M:715:THR:OG1	2:M:718:GLY:O	2.20	0.59
3:N:1108:ARG:NH2	3:N:1198:TYR:O	2.31	0.59
2:C:41:ASN:O	2:C:46:ALA:HB2	2.02	0.59
2:M:872:ASN:ND2	3:N:784:ASP:OD2	2.35	0.59
3:N:643:GLY:HA3	3:N:727:GLN:HB2	1.84	0.59
3:D:1324:PRO:HG3	3:D:1330:ILE:HD11	1.85	0.59
1:L:111:ALA:HB3	1:L:125:PRO:HA	1.84	0.59
3:D:418:GLY:HA2	3:D:428:LYS:HD3	1.83	0.59
1:L:77:GLU:O	1:L:81:ASN:ND2	2.36	0.59
2:M:74:GLY:HA3	2:M:93:PRO:HG2	1.85	0.59
3:N:954:ALA:O	3:N:1062:ARG:NH2	2.35	0.59
3:N:1364:HIS:ND1	3:N:1366:LYS:HG2	2.18	0.59
2:M:808:ARG:NH2	5:P:305:GLU:OE2	2.36	0.59
2:M:628:PHE:H	2:M:638:ASP:CB	2.16	0.58
2:M:35:PRO:HG2	2:M:38:LYS:HB2	1.85	0.58
2:M:936:VAL:HG11	2:M:959:PRO:HB2	1.84	0.58
1:K:48:ILE:HD12	1:K:213:GLN:HG3	1.85	0.58
2:C:397:GLU:HG3	2:C:631:SER:HB2	1.85	0.58
3:N:208:PRO:HA	3:N:390:PRO:HA	1.84	0.58
2:C:937:ASP:OD1	2:C:939:ARG:HD3	2.03	0.58
3:D:1096:ARG:NH1	3:D:1440:PHE:O	2.36	0.58
2:M:680:ASP:OD2	2:M:978:ARG:NH2	2.36	0.58
3:N:57:GLU:HG3	3:N:64:LYS:HB3	1.86	0.58
3:D:904:VAL:HG22	3:D:905:PRO:HD2	1.86	0.58
3:D:486:ARG:HA	3:D:489:ARG:HH21	1.69	0.58
3:N:206:ARG:NH2	5:P:101:GLU:OE2	2.37	0.58
2:C:176:VAL:HG22	2:C:182:VAL:HG12	1.85	0.57
2:M:370:ALA:O	5:P:280:GLN:NE2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1383:ASP:HB3	3:D:1416:ALA:HB3	1.86	0.57
3:N:1211:MET:HE1	4:O:16:LYS:HD2	1.87	0.57
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.87	0.57
3:D:128:TYR:OH	3:D:579:ASP:OD2	2.22	0.57
3:N:1168:MET:HA	3:N:1168:MET:HE3	1.86	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
3:D:1100:ASP:OD2	3:D:1463:LYS:NZ	2.34	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	15: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	15: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:H8	7:H:25:DA:OP2	1.88	0.56
2:M:189:ARG:HH22	2:M:244:PRO:HD3	1.71	0.56
3:N:356:PRO:HG2	3:N:359:ALA:HB2	1.86	0.56
2:C:182:VAL:HG23	2:C:193:LEU:HB3	1.88	0.56
3:N:89:ARG:NH1	15:N:2103:HOH:O	2.33	0.56
3:N:787:LEU:HD21	3:N:947:ILE:HG21	1.88	0.56
2:M:714:ASP:OD2	2:M:808:ARG:NH1	2.39	0.56
3:N:658:LEU:HA	3:N:661:MET:HE3	1.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
13:N:2005:C5P:O2	6:R:15:DG:N2	2.35	0.55
1:A:70:GLY:N	2:C:607:ASP:OD1	2.37	0.55
2:C:405:ARG:HD3	2:C:566:THR:HG21	1.88	0.55
2:M:243:ARG:NH1	7:S:9:DG:O6	2.40	0.55
1:A:20:TYR:OH	1:A:198:ARG:HD2	2.07	0.55
2:C:670:GLN:HG2	2:C:699:PHE:CD2	2.41	0.55
1:K:198:ARG:HD3	2:M:934:PHE:CZ	2.40	0.55
2:M:937:ASP:OD1	2:M:939:ARG:HD3	2.07	0.55
2:M:169:GLY:HA3	2:M:267:TYR:HD1	1.71	0.54
3:N:1324:PRO:HG3	3:N:1330:ILE:HD11	1.88	0.54
1:A:179:PHE:HB3	1:A:197:LEU:HD23	1.88	0.54
2:C:930:LYS:HE3	2:C:935:GLY:HA2	1.90	0.54
1:K:112:ARG:HG3	1:K:125:PRO:HB2	1.88	0.54
3:D:1364:HIS:ND1	3:D:1366:LYS:HG2	2.20	0.54
3:N:1126:ASP:OD2	3:N:1127:GLU:N	2.40	0.54
3:D:241:ILE:HA	3:D:312:ARG:HB3	1.88	0.54
2:M:405:ARG:HD2	2:M:442:GLU:OE2	2.08	0.54
3:N:236:TYR:HB3	3:N:313:MET:HG3	1.90	0.54
3:N:996:TRP:CD2	3:N:1056:PRO:HG3	2.43	0.54
3:N:904:VAL:HG22	3:N:905:PRO:HD2	1.90	0.54
3:N:1236:LEU:HA	3:N:1359:GLN:HG3	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:64:GLU:HA	1:L:165:ILE:HD13	1.89	0.53
1:L:128:HIS:CE1	1:L:131:THR:HG23	2.44	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:N:949:ILE:HD11	3:N:1023:MET:HE1	1.90	0.53
3:D:371:ILE:HG23	5:F:230:LYS:HD2	1.90	0.53
2:M:333:ILE:HD11	2:M:467:ILE:HD11	1.90	0.53
1:B:132:LEU:HD21	1:B:138:LEU:HB2	1.90	0.53
2:C:872:ASN:ND2	3:D:784:ASP:OD1	2.40	0.53
3:D:1426:LYS:O	3:D:1430:SER:OG	2.21	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:936:VAL:HG11	2:C:959:PRO:HB2	1.90	0.53
2:C:1056:LYS:HE2	3:D:751:LEU:HG	1.91	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:232:GLU:HG3	2:C:250:ARG:HE	1.73	0.52
2:C:1050:GLN:O	2:C:1054:THR:OG1	2.21	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:36:LEU:HD11	1:L:221:HIS:HB3	1.93	0.51
1:L:57:TYR:CE1	1:L:163:ASN:HB2	2.46	0.51
3:N:268:ALA:HB3	3:N:284:LEU:HD12	1.93	0.51
3:N:520:LEU:HD12	3:N:521:PRO:HD2	1.93	0.51
3:D:314:PRO:HB2	3:D:317:VAL:HG12	1.93	0.51
2:M:169:GLY:HA3	2:M:267:TYR:CD1	2.46	0.51
2:M:773:LEU:HD23	5:P:354:LEU:HD13	1.93	0.51
1:A:218:LEU:HD23	1:B:222:LEU:HD21	1.91	0.51
2:C:324:ASP:HB3	2:C:327:HIS:HB2	1.93	0.51
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:945:SER:OG	3:D:947:ILE:HG12	2.11	0.50
3:D:1143:GLY:O	3:D:1147:ARG:HD2	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: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:1345:GLU:HG3	3:D:1376:MET:HE3	1.94	0.49
3:D:1444:THR:O	3:D:1448:THR:HG23	2.11	0.49
1:K:219:ARG:HG3	15:L:2111:HOH:O	2.11	0.49
2:M:184:MET:HE1	2:M:196:LEU:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:PRO:HG3	1:B:39:PRO:HG3	1.94	0.49
1:A:150:TYR:CD1	2:C:696:LYS:HG2	2.47	0.49
6:G:16:DT:H3	12:G:101:NAD:H62A	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
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:284:LEU:HD22	3:N:288:MET:HE2	1.94	0.49
3:N:1130:ARG:O	3:N:1131:SER:HB3	2.13	0.49
5:P:131:VAL:HG13	5:P:178:ARG:HD3	1.94	0.49
5:P:152:ASP:N	5:P:152:ASP:OD1	2.45	0.49
2:C:229:MET:HB2	2:C:233:GLU:HB2	1.95	0.49
3:D:1491:THR:O	3:D:1495:ILE:HG13	2.13	0.49
3:N:750:PRO:HG2	3:N:756:GLN:NE2	2.27	0.49
3:D:489:ARG:NH1	3:D:1391:GLU:OE1	2.46	0.49
3:D:801:GLY:O	3:D:804:LEU:HG	2.13	0.49
3:N:366:LYS:HD3	3:N:369:ALA:HB2	1.94	0.49
5:P:193:ARG:HB3	7:S:7:DG:H5"	1.95	0.49
2:C:1042:ALA:HB3	3:D:710:ARG:HB3	1.95	0.49
3:N:208:PRO:HG2	3:N:353:VAL:HG21	1.95	0.49
1:A:57:TYR:CD1	1:A:161:ARG:HD2	2.48	0.48
2:C:711:GLU:HG2	2:C:822:VAL:HG22	1.94	0.48
3:D:218:LYS:HG2	3:D:338:GLU:HG2	1.95	0.48
3:D:959:GLU:HB3	3:D:963:TYR:CE1	2.47	0.48
1:K:56:VAL:HG21	1:K:82:LEU:HD13	1.94	0.48
2:M:397:GLU:HG3	2:M:631:SER:HB2	1.94	0.48
2:M:673:LEU:HD23	2:M:867:VAL:HA	1.95	0.48
2:M:47:ALA:O	2:M:51:THR:HG23	2.12	0.48
2:M:462:ASP:HB3	2:M:468:ARG:HD2	1.94	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	15:M:1306:HOH:O	2.42	0.48
3:N:215:TYR:HE1	3:N:381:ALA:H	1.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:K:218:LEU:HG	1:L:222:LEU:HD11	1.95	0.48
2:M:497:ALA:HB3	2:M:532:MET:HG3	1.94	0.48
2:M:1009:SER:O	3:N:624:ASP:HB3	2.14	0.48
2:C:1102:LEU:HB2	3:D:7:LYS:HB2	1.95	0.48
3:D:208:PRO:HG2	3:D:353:VAL:HG21	1.95	0.48
3:D:227:LEU:HD13	3:D:331:VAL:HB	1.95	0.48
3:D:704:ARG:HB2	3:D:745:MET:HE2	1.96	0.48
1:L:78:ILE:HG21	1:L:140:MET:HE1	1.94	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
2:C:224:GLU:CD	2:C:224:GLU:H	2.21	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
15: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:D:657:LEU:HG	3:D:661:MET:HE2	1.95	0.47
3:N:542:ASP:OD2	3:N:545:ARG:NH2	2.47	0.47
1:L:150:TYR:CE1	1:L:170:VAL:HG22	2.50	0.47
1:L:153:ALA:HA	1:L:156:HIS:NE2	2.29	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:K:70:GLY:H	2:M:607:ASP:CG	2.23	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:71:VAL:HG22	1:L:132:LEU:HG	1.96	0.47
2:M:184:MET:HE3	2:M:186:VAL:HG21	1.97	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
5:P:89:GLY:HA3	7:S:7:DG:C6	2.49	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:N	1:L:113:ASP:OD2	2.48	0.47
2:M:24:GLU:HG3	2:M:27:ARG:HH21	1.79	0.47
3:N:704:ARG:HB2	3:N:745:MET:HE2	1.96	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:40:GLU:OE1	2:M:41:ASN:N	2.48	0.47
2:M:1065:ALA:HB1	2:M:1077:PRO:HG3	1.96	0.47
2:C:28:ARG:NH2	2:C:42:VAL:HG11	2.30	0.46
3:N:1380:GLU:HB2	3:N:1420:LEU:HD22	1.96	0.46
1:A:133:GLU:HG2	1:A:134:GLU:N	2.31	0.46
2:C:63:GLY:HA3	2:C:100:LEU:HD11	1.96	0.46
2:C:595:LEU:HB3	2:C:656:ALA:HB3	1.98	0.46
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.96	0.46
2:M:124:ASP:HB3	2:M:592:LEU:HD12	1.97	0.46
5:P:321:ILE:HD12	5:P:321:ILE:HA	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
1:L:138:LEU:HD21	1:L:140:MET:HE3	1.97	0.46
2:M:859:PRO:O	2:M:867:VAL:HG22	2.16	0.46
3:N:96:ALA:HB3	3:N:554:LEU:HD23	1.98	0.46
3:N:1232:PRO:HG3	3:N:1361:VAL:HG11	1.97	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:372:ASP:HA	3:N:373:PRO:HD3	1.85	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:D:1147:ARG:NH2	3:D:1369:GLU:OE1	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:280:LYS:HE3	2:C:309:TYR:CZ	2.51	0.46
1:K:138:LEU:HD21	1:K:140:MET:HE2	1.98	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
2:M:184:MET:HE2	2:M:191:PHE:CZ	2.51	0.46
3:N:128:TYR:OH	3:N:579:ASP:OD2	2.28	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:633:VAL:C	3:N:635:PRO:HD3	2.41	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:81:THR:OG1	3:D:82:LYS:N	2.49	0.45
3:D:271:VAL:HG22	3:D:281:THR:HG23	1.96	0.45
3:D:1084:THR:O	3:D:1088:THR:HG23	2.16	0.45
2:M:195:LEU:O	2:M:199:VAL:HG23	2.17	0.45
2:M:420:ARG:C	2:M:422:ARG:H	2.24	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:685:ASP:HA	3:N:688:TRP:HD1	1.81	0.45
3:N:1101:VAL:HG13	3:N:1102:THR:HG23	1.97	0.45
3:D:1344:VAL:HB	3:D:1376:MET:HE1	1.98	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:OP2	7:H:25:DA:C8	2.69	0.45
3:N:536:ALA:HA	5:P:315:VAL:O	2.17	0.45
4:O:48:MET:HE2	4:O:48:MET:HB3	1.90	0.45
3:D:409:VAL:HG13	3:D:435:VAL:HG11	1.97	0.45
3:D:1480:PHE:O	4:E:18:ARG:NH2	2.50	0.45
2:M:12:VAL:HG11	2:M:472:ARG:HD3	1.98	0.45
2:M:274:ARG:HH12	2:M:286:SER:C	2.24	0.45
2:M:1083:GLU:OE1	2:M:1086:ARG:NH1	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:185:ARG:NH1	1:L:187:GLY:O	2.50	0.45
2:M:11:GLU:OE2	2:M:537:LYS:HE2	2.17	0.45
2:M:343:GLN:HG3	2:M:385:PHE:HB2	1.99	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:H	5:P:142:ARG:HE	1.62	0.45
3:D:307:ALA:HB1	3:D:311:LEU:HD21	1.98	0.45
3:D:963:TYR:CD2	3:D:1002:LYS:HD3	2.52	0.45
4:E:51:LEU:HD12	4:E:51:LEU:H	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
1:B:78:ILE:HG21	1:B:140:MET:HE1	1.98	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	15: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
2:C:905:ILE:C	2:C:907:ASP:H	2.25	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
2:M:578:VAL:HG23	2:M:671:ASN:CG	2.42	0.45
3:N:162:ARG:O	3:N:449:SER:HB2	2.17	0.45
3:N:243:ALA:HB3	3:N:311:LEU:HD12	1.99	0.45
3:N:473:LEU:HD21	3:N:495:ARG:HH21	1.82	0.45
3:N:729:HIS:O	3:N:732:VAL:HG22	2.17	0.45
2:C:36:PRO:HB3	2:C:70:GLU:HB2	1.98	0.45
1:K:105:GLY:O	1:K:107:LYS:N	2.49	0.45
2:M:778:PHE:CD1	5:P:422:LEU:HD22	2.52	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
3:N:1143:GLY:O	3:N:1147:ARG:HD2	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:142:ARG:HE	5:P:142:ARG:N	2.15	0.44
5:P:212:LEU:HD22	5:P:247:ILE:HG23	1.99	0.44
2:C:146:VAL:HG22	2:C:162:ILE:HG12	2.00	0.44
3:D:235:ALA:HA	3:D:322:VAL:HG23	1.99	0.44
3:D:637:LEU:HD13	3:D:642:CYS:HA	1.99	0.44
2:M:561:GLY:O	2:M:565:GLN:HG3	2.17	0.44
2:C:1037:VAL:HG13	2:C:1049:LEU:HD11	1.98	0.44
1:L:220:GLU:O	1:L:223:THR:OG1	2.24	0.44
2:M:76:PRO:HA	2:M:77:PRO:HD2	1.89	0.44
2:M:243:ARG:HH12	7:S:9:DG:H1	1.64	0.44
2:M:1035:MET:HE2	3:N:707:THR:O	2.17	0.44
3:N:307:ALA:HB1	3:N:311:LEU:HD21	1.99	0.44
3:N:1314:LYS:HG3	3:N:1317:ASP:OD2	2.18	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:HA	5:F:88:ILE:HD12	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
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
3:D:658:LEU:HA	3:D:661:MET:HE3	1.99	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:617:ASP:OD2	2:C:619:ARG:HG2	2.17	0.44
2:C:1110:ASP:OD2	2:C:1114:GLY:N	2.43	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: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	15:P:2103:HOH:O	2.17	0.44
2:C:397:GLU:H	2:C:633:GLN:NE2	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:33:ASP:HB2	15:C:1386:HOH:O	2.17	0.43
2:C:1090:LYS:HA	2:C:1090:LYS:HD3	1.85	0.43
3:D:561:GLY:HA3	5:F:132:ARG:HD3	2.00	0.43
1:K:83:LYS:NZ	2:M:698:ASP:OD1	2.51	0.43
1:K:97:VAL:HG12	1:K:99:LEU:HD12	1.98	0.43
2:M:23:VAL:HA	2:M:121:MET:SD	2.57	0.43
2:M:937:ASP:OD2	2:M:939:ARG:NH1	2.50	0.43
3:N:1266:ARG:HD3	7:S:19:DG:H5"	1.99	0.43
5:P:172:ARG:O	5:P:176:ILE:HG12	2.17	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:805:ARG:O	2:C:807:ARG:NH2	2.51	0.43
2:C:1065:ALA:CB	2:C:1077:PRO:HG3	2.48	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:626:ARG:HG3	2:C:629:TYR:CD2	2.53	0.43
2:C:1031:ARG:HG2	6:G:16:DT:H5"	2.01	0.43
3:D:90:MET:HE3	3:D:90:MET:HB3	1.92	0.43
3:D:200:ASP:O	3:D:397:LYS:HG2	2.18	0.43
5:F:259:ARG:HD2	15: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:HD23	2:M:944:LEU:HA	1.86	0.43
3:N:520:LEU:O	3:N:525:ARG:NE	2.50	0.43
1:B:128:HIS:HE1	1:B:131:THR:HG23	1.83	0.43
2:C:884:GLN:O	2:C:888:THR:OG1	2.29	0.43
3:D:185:VAL:N	3:D:201:GLY:O	2.40	0.43
3:D:411:THR:O	5:F:178:ARG:NH1	2.44	0.43
3:D:573:MET:SD	5:F:210:LEU:HB3	2.58	0.43
3:D:633:VAL:C	3:D:635:PRO:HD3	2.44	0.43
3:D:966:GLU:O	3:D:969:ARG:HB3	2.18	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
1:K:66:SER:HB2	1:K:75:VAL:HG21	2.00	0.43
2:M:26:TYR:OH	2:M:119:PRO:O	2.36	0.43
3:N:654:LYS:O	3:N:658:LEU:HG	2.19	0.43
3:N:1312:LEU:HD12	3:N:1324:PRO:HB2	2.01	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:HB3	3:N:180:LYS:HE2	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:OD1	2:C:881:ASN:N	2.52	0.42
3:D:1420:LEU:HD12	3:D:1420:LEU:HA	1.88	0.42
3:D:1488:ASP:OD1	15:D:2102:HOH:O	2.21	0.42
4:E:13:VAL:HG21	4:E:19:LEU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:172:ARG:O	5:F:176:ILE:HG12	2.19	0.42
5:F:226:LYS:HB3	5:F:226:LYS:HE3	1.74	0.42
2:M:1090:LYS:NZ	15:M:1309:HOH:O	2.48	0.42
3:N:95:LEU:HA	3:N:551:ASN:HD21	1.84	0.42
3:N:236:TYR:CZ	3:N:242:LEU:HD12	2.54	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	15: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	15:C:1335:HOH:O	2.19	0.42
2:C:984:GLU:OE2	3:D:791:TYR:OH	2.30	0.42
2:M:905:ILE:C	2:M:907:ASP:H	2.27	0.42
3:N:401:TYR:OH	3:N:430:ASP:OD2	2.33	0.42
2:C:226:VAL:HA	2:C:229:MET:HE3	2.02	0.42
2:C:359:MET:HG2	2:C:372:LEU:HD22	2.01	0.42
3:D:68:PHE:O	3:D:71:LYS:HB3	2.19	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: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:HD23	2:C:328:LEU:HA	1.87	0.42
3:D:241:ILE:HD11	3:D:310:LEU:HB3	2.02	0.42
3:D:1485:GLN:O	4:E:75:PHE:HA	2.20	0.42
2:M:328:LEU:HA	2:M:328:LEU:HD23	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
2:C:922:PHE:CE2	2:C:964:LYS:HB2	2.55	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
3:D:1461:GLY:O	3:D:1465:ASN:ND2	2.51	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
13:N:2005:C5P:C2	6:R:15:DG:H22	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:540:LEU:HD23	3:D:540:LEU:HA	1.92	0.42
3:D:659:LYS:HA	3:D:659:LYS:HD2	1.90	0.42
3:D:971:LEU:HD22	3:D:971:LEU:HA	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:38:LYS:HA	3:D:38:LYS:HD3	1.68	0.42
3:D:140:ALA:HA	3:D:450:TYR:CD2	2.55	0.42
3:D:159:ARG:NH2	15:D:2123:HOH:O	2.52	0.42
3:D:711:LEU:HD13	3:D:778:LEU:HD23	2.02	0.42
5:F:110:MET:HE2	5:F:110:MET:HB3	1.89	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:648:MET:HE2	3:N:648:MET:HB3	1.93	0.42
3:D:970:LYS:O	3:D:974:ILE:HG12	2.19	0.41
3:D:1137:ARG:O	3:D:1141:GLU:HG3	2.19	0.41
5:F:333:ILE:HA	5:F:334:PRO:HD3	1.86	0.41
2:M:29:ALA:O	2:M:44:ILE:HG22	2.20	0.41
2:M:249:LYS:HB2	2:M:249:LYS:HE3	1.70	0.41
2:M:674:VAL:O	2:M:989:VAL:HA	2.20	0.41
3:N:684:LYS:HE2	3:N:684:LYS:HB3	1.79	0.41
3:N:1130:ARG:O	3:N:1130:ARG:NE	2.53	0.41
3:N:1292:VAL:HG23	3:N:1305:LEU:HD21	2.02	0.41
2:C:43:GLY:O	2:C:46:ALA:HB3	2.20	0.41
3:D:661:MET:HE3	3:D:673:ALA:HB1	2.02	0.41
3:D:1362:LYS:HB2	3:D:1362:LYS:HE2	1.89	0.41
5:F:80:PRO:HB2	5:F:210:LEU:HD11	2.02	0.41
5:F:153:PRO:HA	5:F:156:VAL:HG22	2.01	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	15:D:2240:HOH:O	2.19	0.41
5:F:326:ASP:OD1	5:F:326:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:66:GLN:HE21	3:N:66:GLN:HB2	1.57	0.41
3:N:115:LEU:HD23	3:N:115:LEU:HA	1.95	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:353:VAL:HG11	3:D:387:LEU:HD11	2.03	0.41
3:D:527:MET:HB2	3:D:527:MET:HE2	1.68	0.41
3:D:1307:LYS:H	3:D:1307:LYS:HG3	1.70	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	15:M:1301:HOH:O	2.19	0.41
3:N:54:LYS:HB3	3:N:54:LYS:NZ	2.36	0.41
3:N:544:TYR:O	3:N:548:ILE:HG13	2.21	0.41
3:N:961:LYS:HE3	3:N:961:LYS:HB2	1.90	0.41
3:N:1487:VAL:HG22	3:N:1491:THR:HB	2.01	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: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
3:D:1264:GLU:OE2	3:D:1425:THR:OG1	2.38	0.41
1:L:115:LEU:HA	1:L:116:PRO:HD3	1.91	0.41
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:149:LYS:HB3	3:D:149:LYS:HE3	1.91	0.41
3:D:1147:ARG:HH22	3:D:1369:GLU:CD	2.29	0.41
3:D:1150:ALA:HB3	3:D:1187:PRO:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:M:778:PHE:CZ	5:P:419:ARG:HA	2.56	0.41
3:N:841:TYR:HB2	3:N:864:VAL:CG2	2.51	0.41
3:N:1147:ARG:HH22	3:N:1369:GLU:CD	2.25	0.41
1:A:9:PRO:HB3	1:A:27:PRO:O	2.20	0.41
1:A:216:GLU:CD	1:A:219:ARG:HH21	2.29	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:76:PRO:HG3	2:C:120:LEU:CD1	2.50	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
3:D:372:ASP:HB3	3:D:374:GLU:OE2	2.21	0.41
3:D:1144:LEU:HA	3:D:1144:LEU:HD23	1.86	0.41
4:E:30:LEU:HA	4:E:30:LEU:HD23	1.83	0.41
4:E:31:LEU:HD23	4:E:31:LEU:HA	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:K:70:GLY:N	2:M:607:ASP:OD1	2.54	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:13:ILE:HG13	2:M:458:TYR:HE2	1.84	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
3:N:935:LYS:HE2	3:N:935:LYS:HB3	1.94	0.41
3:N:1373:ARG:HD3	15:N:2204:HOH:O	2.21	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:20:TYR:C	1:K:207:PRO:HG2	2.46	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
2:M:764:GLU:H	2:M:764:GLU:HG3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:LEU:O	1:B:83:LYS:HB2	2.21	0.40
1:B:150:TYR:CE1	1:B:170:VAL:HG22	2.56	0.40
2:C:76:PRO:HA	2:C:77:PRO:HD2	1.88	0.40
2:C:599:GLU:HG3	2:C:600:ASP:H	1.86	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:708:LEU:HA	3:N:708:LEU:HD23	1.85	0.40
3:N:1378:TYR:CZ	3:N:1430:SER:HB2	2.57	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
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
3:N:1379:VAL:HG21	3:N:1400:VAL:HG11	2.03	0.40
4:O:9:LEU:HD23	4:O:9:LEU:HA	1.93	0.40
4:O:83:ASP:O	4:O:87:LYS:HG2	2.21	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:HD23	3:N:468:LEU:HA	1.89	0.40
3:N:671:LYS:NZ	5:P:421:PHE:HA	2.37	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:685:ASP:HA	3:D:688:TRP:HD1	1.87	0.40
2:M:775:ARG:CZ	2:M:782:ALA:HB2	2.52	0.40
2:M:1102:LEU:HD23	2:M:1108:PRO:HA	2.03	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
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
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
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%)	48	80
4	E	92/99 (93%)	90 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	32	65
1	B	195/273 (71%)	188 (96%)	7 (4%)	31	65
1	K	199/273 (73%)	190 (96%)	9 (4%)	24	59
1	L	195/273 (71%)	190 (97%)	5 (3%)	40	72
2	C	933/941 (99%)	896 (96%)	37 (4%)	28	62
2	M	917/941 (97%)	872 (95%)	45 (5%)	22	56
3	D	1252/1279 (98%)	1188 (95%)	64 (5%)	21	55
3	N	1251/1279 (98%)	1189 (95%)	62 (5%)	22	56
4	E	82/88 (93%)	76 (93%)	6 (7%)	13	42
4	O	82/88 (93%)	78 (95%)	4 (5%)	22	56
5	F	301/388 (78%)	292 (97%)	9 (3%)	36	69
5	P	277/388 (71%)	256 (92%)	21 (8%)	12	41
All	All	5883/6484 (91%)	5607 (95%)	276 (5%)	23	58

All (276) 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	51	THR
1	B	154	GLU
1	B	180	GLN
1	B	184	THR
1	B	197	LEU
2	C	194	VAL
2	C	210	GLU
2	C	211	LEU
2	C	216	GLU
2	C	217	LEU
2	C	222	MET
2	C	246	ASP
2	C	261	ILE
2	C	265	ARG
2	C	276	LYS
2	C	284	ARG
2	C	285	LEU
2	C	358	ARG
2	C	360	LEU
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
2	C	490	GLU
2	C	513	VAL
2	C	530	GLU
2	C	610	ARG
2	C	617	ASP
2	C	670	GLN
2	C	766	GLU
2	C	807	ARG

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Mol	Chain	Res	Type
2	C	815	LEU
2	C	816	LYS
2	C	830	LYS
2	C	939	ARG
2	C	952	LEU
2	C	978	ARG
2	C	1080	SER
2	C	1117	SER
3	D	30	GLU
3	D	35	ARG
3	D	67	ARG
3	D	71	LYS
3	D	106	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	242	LEU
3	D	273	ARG
3	D	293	VAL
3	D	311	LEU
3	D	312	ARG
3	D	346	ARG
3	D	354	VAL
3	D	374	GLU
3	D	387	LEU
3	D	407	VAL
3	D	409	VAL
3	D	415	VAL
3	D	442	ASN
3	D	471	GLU
3	D	508	ARG
3	D	527	MET
3	D	611	GLN
3	D	618	LEU
3	D	632	VAL
3	D	687	VAL
3	D	694	VAL
3	D	709	HIS
3	D	710	ARG

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Mol	Chain	Res	Type
3	D	754	PHE
3	D	778	LEU
3	D	784	ASP
3	D	808	THR
3	D	864	VAL
3	D	875	THR
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	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	1253	THR
3	D	1267	ARG
3	D	1280	VAL
3	D	1290	LEU
3	D	1295	GLU
3	D	1389	LEU
3	D	1430	SER
3	D	1486	VAL
4	E	31	LEU
4	E	51	LEU
4	E	52	GLU
4	E	55	PHE
4	E	80	VAL
4	E	92	LEU
5	F	88	ILE
5	F	150	THR
5	F	193	ARG
5	F	205	ARG
5	F	279	GLN
5	F	324	GLU

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Mol	Chain	Res	Type
5	F	346	THR
5	F	416	ARG
5	F	420	ASP
1	K	6	LEU
1	K	10	VAL
1	K	74	ASP
1	K	96	THR
1	K	126	ASP
1	K	142	VAL
1	K	184	THR
1	K	196	THR
1	K	227	ASN
1	L	10	VAL
1	L	67	THR
1	L	96	THR
1	L	113	ASP
1	L	145	ASP
2	M	20	GLU
2	M	42	VAL
2	M	44	ILE
2	M	49	ARG
2	M	51	THR
2	M	54	ILE
2	M	113	VAL
2	M	149	THR
2	M	165	LEU
2	M	184	MET
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	261	ILE
2	M	276	LYS
2	M	284	ARG
2	M	294	GLU
2	M	336	VAL
2	M	358	ARG
2	M	388	ARG

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Mol	Chain	Res	Type
2	M	402	SER
2	M	409	ARG
2	M	438	ILE
2	M	454	SER
2	M	504	GLU
2	M	513	VAL
2	M	566	THR
2	M	637	LEU
2	M	670	GLN
2	M	705	ILE
2	M	730	SER
2	M	768	THR
2	M	771	GLU
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	69	GLU
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	279	VAL
3	N	310	LEU
3	N	317	VAL
3	N	340	THR
3	N	367	ILE
3	N	374	GLU
3	N	378	ILE
3	N	400	VAL
3	N	420	VAL
3	N	421	LEU

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Mol	Chain	Res	Type
3	N	430	ASP
3	N	456	MET
3	N	618	LEU
3	N	628	ARG
3	N	632	VAL
3	N	650	LEU
3	N	687	VAL
3	N	694	VAL
3	N	724	GLN
3	N	725	SER
3	N	753	SER
3	N	754	PHE
3	N	778	LEU
3	N	810	GLU
3	N	838	ARG
3	N	864	VAL
3	N	904	VAL
3	N	956	ILE
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	1128	VAL
3	N	1130	ARG
3	N	1132	LEU
3	N	1154	GLU
3	N	1188	VAL
3	N	1282	ARG
3	N	1284	GLU
3	N	1299	PHE
3	N	1307	LYS
3	N	1314	LYS
3	N	1455	LYS
3	N	1486	VAL
3	N	1487	VAL
3	N	1493	LYS
3	N	1497	GLU
3	N	1500	LYS
4	O	80	VAL
4	O	82	GLU

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Mol	Chain	Res	Type
4	O	83	ASP
4	O	93	TYR
5	P	95	THR
5	P	135	ILE
5	P	140	ARG
5	P	142	ARG
5	P	149	GLU
5	P	150	THR
5	P	151	LEU
5	P	156	VAL
5	P	271	LEU
5	P	277	GLN
5	P	315	VAL
5	P	319	THR
5	P	321	ILE
5	P	323	ASP
5	P	346	THR
5	P	367	MET
5	P	369	LEU
5	P	396	ARG
5	P	403	LYS
5	P	419	ARG
5	P	423	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	99	GLN
2	C	102	HIS
2	C	117	HIS
2	C	390	GLN
2	C	633	GLN
2	C	860	HIS
2	C	962	GLN
2	C	1047	HIS
2	C	1107	ASN
3	D	66	GLN
3	D	348	GLN
3	D	442	ASN
3	D	560	GLN
3	D	696	HIS
3	D	703	ASN

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Mol	Chain	Res	Type
3	D	901	GLN
3	D	994	GLN
3	D	1014	ASN
3	D	1037	GLN
3	D	1046	GLN
3	D	1116	ASN
3	D	1124	GLN
3	D	1184	GLN
3	D	1359	GLN
5	F	83	GLN
5	F	175	HIS
5	F	185	GLN
1	K	38	ASN
1	K	63	HIS
1	K	188	GLN
1	L	63	HIS
2	M	31	GLN
2	M	204	GLN
2	M	219	GLN
2	M	390	GLN
2	M	448	ASN
2	M	500	ASN
2	M	663	ASN
2	M	991	GLN
2	M	1107	ASN
3	N	66	GLN
3	N	616	GLN
3	N	724	GLN
3	N	994	GLN
3	N	1014	ASN
3	N	1046	GLN
3	N	1116	ASN
3	N	1124	GLN
3	N	1172	HIS
3	N	1184	GLN
4	O	86	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 oligosaccharides 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	1.77	1 (16%)	12,13,47	1.01	0
11	CTP	M	1201	8	6,8,30	1.11	1 (16%)	12,13,47	0.89	0
10	C	D	2005	8,12	18,21,22	0.25	0	25,30,33	0.37	0
12	NAD	G	101	10	46,48,48	2.02	13 (28%)	64,73,73	1.39	7 (10%)
14	AMP	R	101	13	25,25,25	1.92	9 (36%)	37,38,38	1.45	2 (5%)
13	C5P	N	2005	8,14	18,21,22	0.26	0	25,30,33	0.34	0

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	-
10	C	D	2005	8,12	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	NAD	G	101	10	-	10/30/62/62	0/5/5/5
14	AMP	R	101	13	-	5/10/26/26	0/3/3/3
13	C5P	N	2005	8,14	-	0/7/25/26	0/2/2/2

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	G	101	NAD	C7N-N7N	6.14	1.44	1.33
12	G	101	NAD	O4D-C1D	5.81	1.48	1.40
11	D	2006	CTP	PA-O1A	3.90	1.62	1.50
14	R	101	AMP	C6-N6	3.78	1.43	1.34
12	G	101	NAD	C6A-N6A	3.66	1.43	1.34
14	R	101	AMP	C2-N1	3.64	1.40	1.33
12	G	101	NAD	C2A-N1A	3.52	1.40	1.33
14	R	101	AMP	C1'-N9	3.24	1.55	1.46
14	R	101	AMP	C2-N3	3.19	1.39	1.33
12	G	101	NAD	C2A-N3A	3.19	1.39	1.33
14	R	101	AMP	O4'-C1'	3.09	1.49	1.42
12	G	101	NAD	C1B-N9A	3.04	1.54	1.46
12	G	101	NAD	O4B-C1B	3.02	1.49	1.42
12	G	101	NAD	O2D-C2D	-2.71	1.36	1.43
12	G	101	NAD	O2B-C2B	-2.38	1.37	1.43
14	R	101	AMP	O2'-C2'	-2.32	1.37	1.43
12	G	101	NAD	C5A-C6A	-2.19	1.34	1.41
11	M	1201	CTP	PA-O5'	2.15	1.62	1.54
12	G	101	NAD	C2B-C3B	-2.15	1.47	1.53
14	R	101	AMP	C8-N7	2.11	1.35	1.31
14	R	101	AMP	C2'-C3'	-2.09	1.47	1.53
14	R	101	AMP	C5-C6	-2.09	1.35	1.41
12	G	101	NAD	O3D-C3D	-2.06	1.37	1.43
12	G	101	NAD	C8A-N7A	2.06	1.35	1.31

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	R	101	AMP	O4'-C1'-N9	5.50	118.65	108.09
12	G	101	NAD	O4B-C1B-N9A	5.36	118.37	108.09
14	R	101	AMP	N3-C2-N1	-4.74	121.41	128.58
12	G	101	NAD	N3A-C2A-N1A	-4.70	121.47	128.58
12	G	101	NAD	C4D-O4D-C1D	-4.02	106.24	109.92
12	G	101	NAD	C3N-C7N-N7N	3.05	121.49	117.74
12	G	101	NAD	C2D-C3D-C4D	2.53	107.50	102.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	G	101	NAD	O7N-C7N-N7N	-2.49	119.02	122.62
12	G	101	NAD	C6N-N1N-C2N	-2.01	120.17	121.88

There are no chirality outliers.

All (15) torsion outliers are listed below:

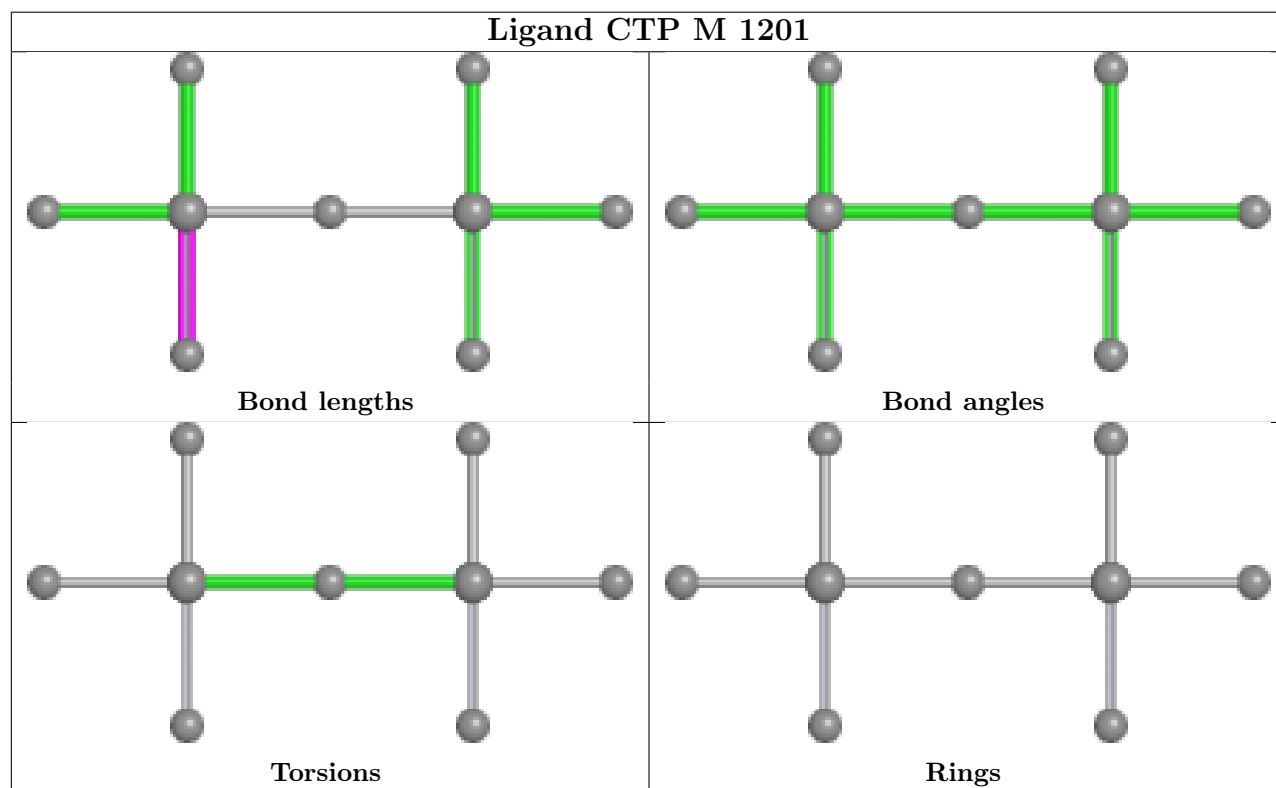
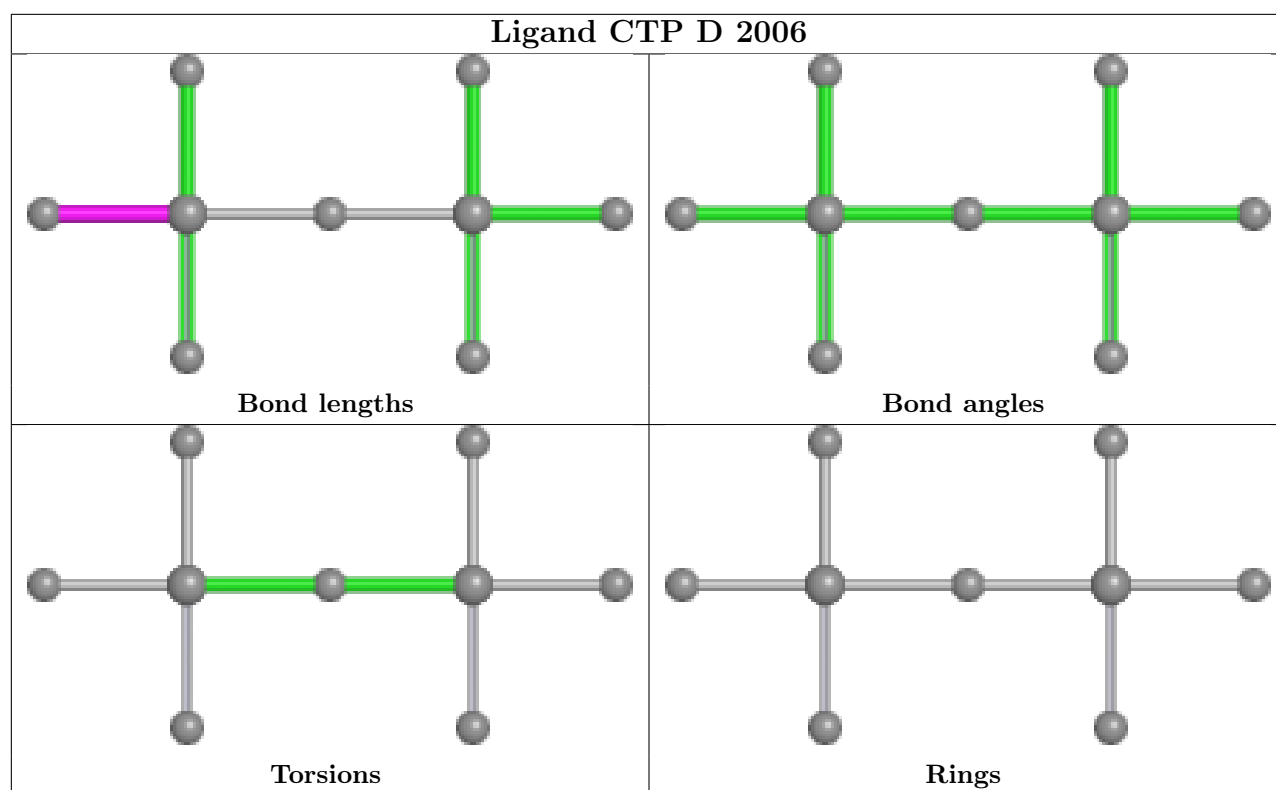
Mol	Chain	Res	Type	Atoms
12	G	101	NAD	C5B-O5B-PA-O2A
12	G	101	NAD	C5B-O5B-PA-O3
12	G	101	NAD	PN-O3-PA-O5B
12	G	101	NAD	O4B-C4B-C5B-O5B
12	G	101	NAD	C5D-O5D-PN-O3
12	G	101	NAD	C5D-O5D-PN-O2N
14	R	101	AMP	C5'-O5'-P-O1P
14	R	101	AMP	C5'-O5'-P-O2P
14	R	101	AMP	O4'-C4'-C5'-O5'
14	R	101	AMP	C3'-C4'-C5'-O5'
12	G	101	NAD	C3B-C4B-C5B-O5B
14	R	101	AMP	C5'-O5'-P-O3P
12	G	101	NAD	C5D-O5D-PN-O1N
12	G	101	NAD	PN-O3-PA-O1A
12	G	101	NAD	PN-O3-PA-O2A

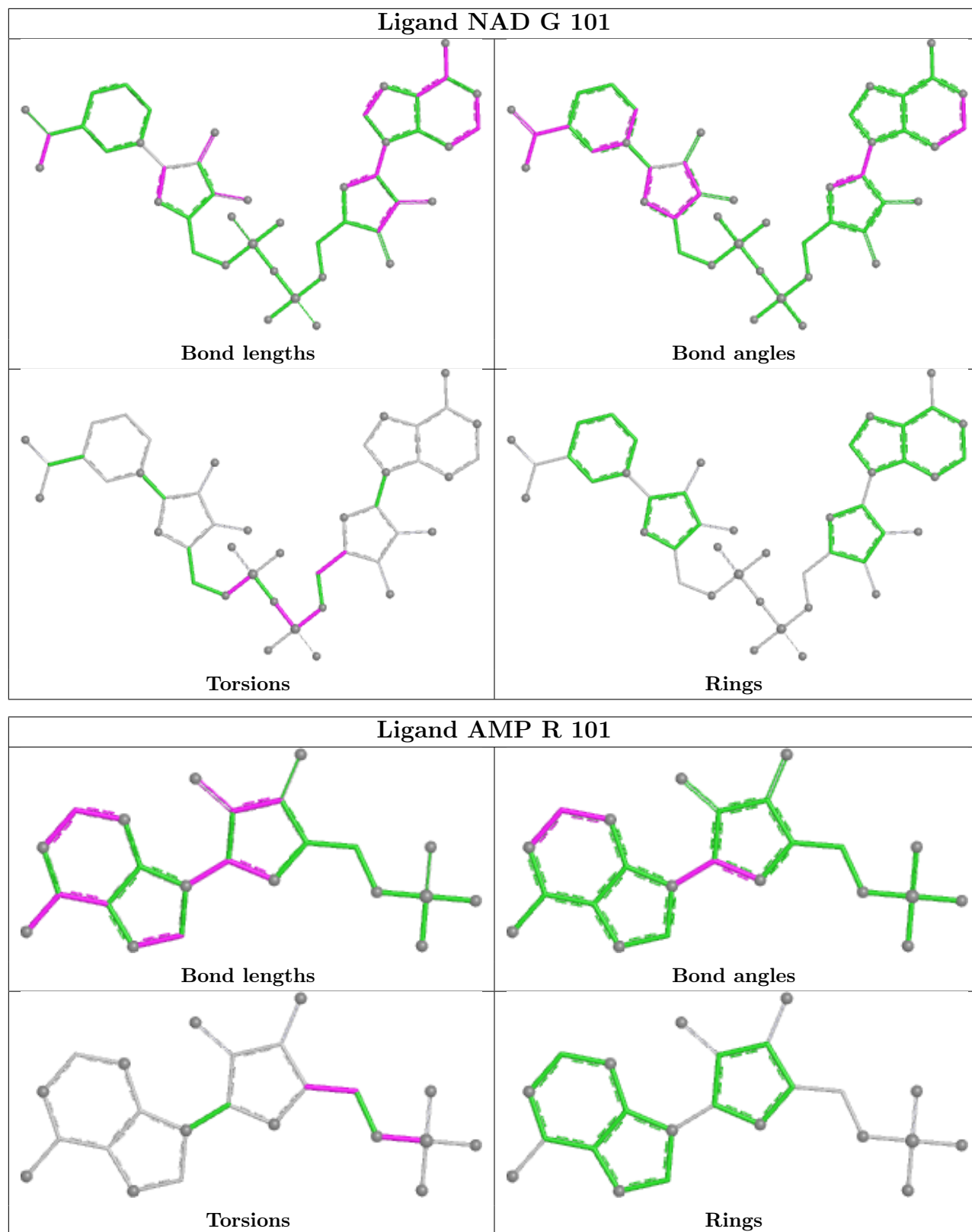
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	G	101	NAD	1	0
13	N	2005	C5P	3	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 ⓘ

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	229/315 (72%)	-0.39	1 (0%) 88 76	7, 21, 48, 79	1 (0%)
1	B	222/315 (70%)	-0.18	1 (0%) 87 72	6, 31, 64, 81	0
1	K	228/315 (72%)	-0.06	4 (1%) 67 44	10, 31, 57, 71	1 (0%)
1	L	222/315 (70%)	-0.02	0 100 100	12, 36, 73, 103	0
2	C	1108/1119 (99%)	-0.43	4 (0%) 88 76	0, 14, 62, 89	3 (0%)
2	M	1091/1119 (97%)	0.26	51 (4%) 36 19	1, 39, 97, 116	2 (0%)
3	D	1485/1524 (97%)	-0.34	7 (0%) 87 72	0, 18, 68, 102	4 (0%)
3	N	1483/1524 (97%)	-0.22	9 (0%) 85 69	0, 24, 77, 106	4 (0%)
4	E	94/99 (94%)	-0.41	0 100 100	1, 13, 49, 67	0
4	O	94/99 (94%)	-0.32	1 (1%) 78 57	4, 23, 62, 71	0
5	F	346/443 (78%)	-0.25	0 100 100	3, 26, 68, 84	0
5	P	316/443 (71%)	0.33	14 (4%) 39 21	17, 46, 91, 109	0
6	G	16/19 (84%)	0.26	1 (6%) 26 13	16, 48, 112, 117	0
6	R	16/19 (84%)	0.72	1 (6%) 26 13	39, 58, 115, 122	0
7	H	21/27 (77%)	0.41	1 (4%) 35 19	19, 56, 108, 124	0
7	S	21/27 (77%)	0.74	1 (4%) 35 19	33, 84, 121, 144	0
All	All	6992/7722 (90%)	-0.17	96 (1%) 73 51	0, 26, 78, 144	15 (0%)

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	P	366	ALA	4.5
2	M	200	LEU	4.5
2	M	807	ARG	4.4
2	C	102	HIS	4.3
2	M	196	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	139	ASN	3.9
3	N	674	ARG	3.8
5	P	371	LEU	3.7
5	P	397	ILE	3.7
5	P	325	LYS	3.7
2	M	247	PRO	3.6
1	K	139	ASN	3.5
3	N	412	GLY	3.4
2	M	66	LEU	3.3
2	M	765	SER	3.1
2	M	63	GLY	3.0
2	M	360	LEU	3.0
2	M	52	PHE	3.0
3	N	184	GLU	2.9
6	R	4	DT	2.8
2	M	270	GLY	2.8
2	M	207	LEU	2.8
2	M	741	GLY	2.7
5	P	368	VAL	2.7
7	S	11	DG	2.7
2	M	51	THR	2.7
2	M	169	GLY	2.7
6	G	4	DT	2.7
3	D	184	GLU	2.7
3	N	311	LEU	2.7
2	M	258	TYR	2.7
5	P	369	LEU	2.7
3	D	1053	PHE	2.6
2	M	638	ASP	2.6
3	D	674	ARG	2.6
2	M	344	PHE	2.6
2	M	188	LYS	2.6
2	M	202	TYR	2.6
2	M	199	VAL	2.6
2	M	340	MET	2.6
2	M	1084	SER	2.5
2	M	176	VAL	2.5
5	P	142	ARG	2.5
2	M	396	ASP	2.5
2	M	769	PRO	2.5
3	N	309	GLY	2.5
3	N	307	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
2	M	217	LEU	2.5
2	M	228	ALA	2.5
2	M	767	PRO	2.4
2	M	236	ILE	2.4
2	M	194	VAL	2.4
2	C	807	ARG	2.3
2	M	255	ALA	2.3
2	M	293	PHE	2.3
7	H	11	DG	2.3
1	K	130	ALA	2.2
5	P	417	LYS	2.2
2	M	291	ALA	2.2
3	N	177	ALA	2.2
5	P	405	LEU	2.2
2	M	275	TYR	2.2
3	N	1053	PHE	2.2
2	M	214	TYR	2.2
3	D	1499	ARG	2.2
2	M	272	ALA	2.2
2	M	191	PHE	2.2
2	M	65	VAL	2.1
5	P	367	MET	2.1
2	M	287	GLY	2.1
2	M	369	PRO	2.1
2	M	181	VAL	2.1
3	D	1129	THR	2.1
2	M	166	PRO	2.1
3	D	175	VAL	2.1
2	M	195	LEU	2.1
2	M	351	LEU	2.1
3	N	378	ILE	2.1
1	K	231	ALA	2.1
1	B	157	GLY	2.1
4	O	95	VAL	2.1
2	M	68	PHE	2.1
2	M	298	PHE	2.1
3	D	1405	GLU	2.1
2	C	64	LEU	2.0
1	K	111	ALA	2.0
2	M	67	ASP	2.0
5	P	410	TYR	2.0
5	P	356	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
2	M	378	LEU	2.0
2	C	361	MET	2.0
5	P	275	ALA	2.0
2	M	254	VAL	2.0
5	P	141	VAL	2.0
2	M	64	LEU	2.0
2	M	283	ILE	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 oligosaccharides 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.

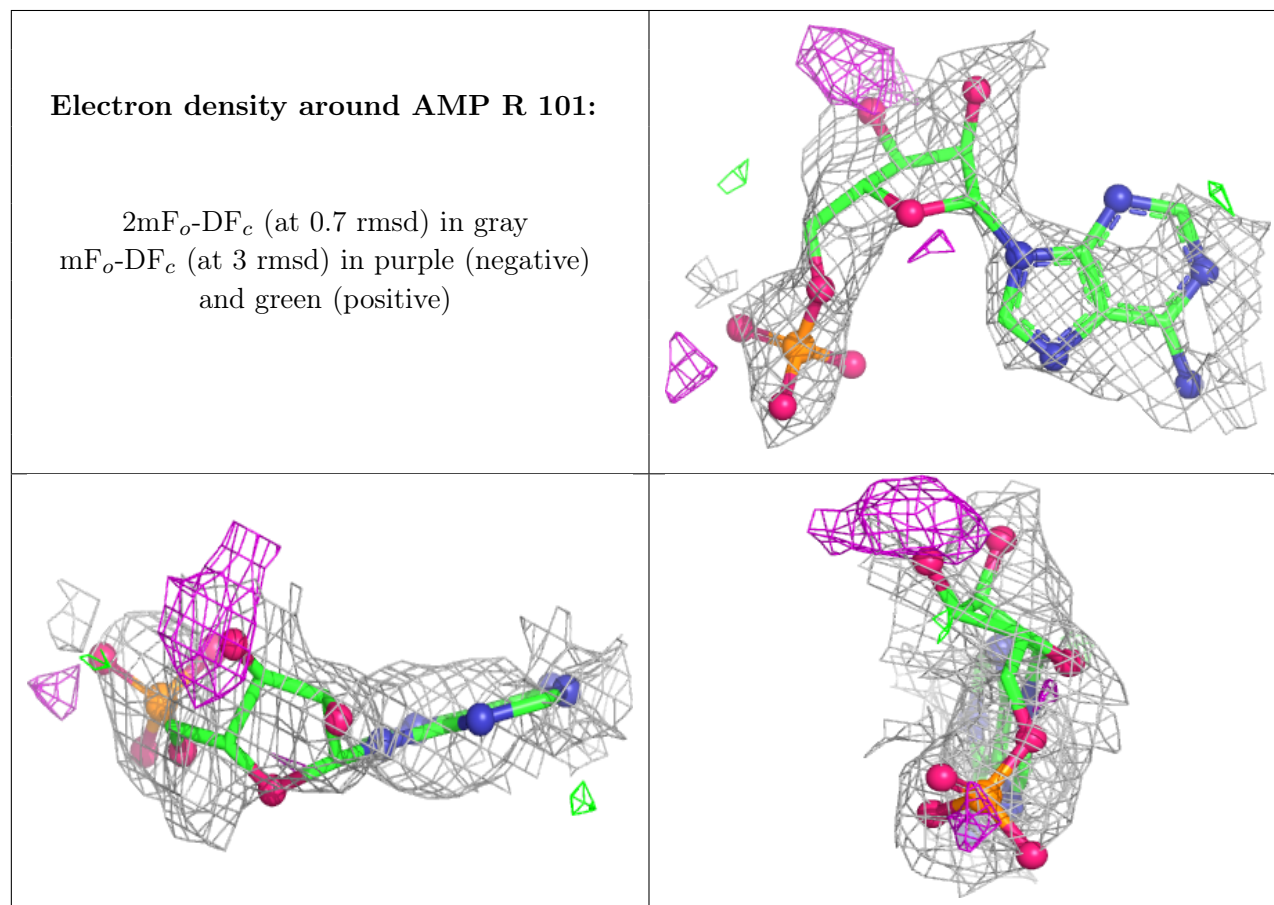
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
14	AMP	R	101	23/23	0.70	0.17	37,54,63,83	23
12	NAD	G	101	44/44	0.81	0.22	15,34,53,67	44
11	CTP	M	1201	9/29	0.83	0.12	25,52,69,73	0
13	C5P	N	2005	20/21	0.84	0.16	22,46,53,59	20
8	MG	P	2001	1/1	0.87	0.08	51,51,51,51	0
11	CTP	D	2006	9/29	0.87	0.10	21,41,62,80	0
8	MG	B	2001	1/1	0.90	0.10	17,17,17,17	0
10	C	D	2005	20/21	0.91	0.12	6,19,38,47	20
8	MG	D	2007	1/1	0.91	0.17	28,28,28,28	0
8	MG	L	2001	1/1	0.93	0.05	41,41,41,41	0
8	MG	F	2001	1/1	0.93	0.07	25,25,25,25	0
8	MG	N	2006	1/1	0.94	0.08	32,32,32,32	0
8	MG	N	2003	1/1	0.95	0.13	6,6,6,6	0
9	ZN	N	2002	1/1	0.96	0.08	89,89,89,89	0
8	MG	N	2004	1/1	0.98	0.04	27,27,27,27	0
8	MG	D	2003	1/1	0.98	0.13	1,1,1,1	0

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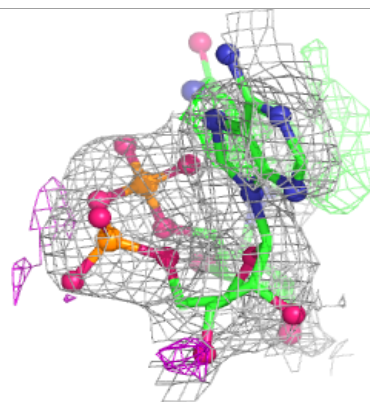
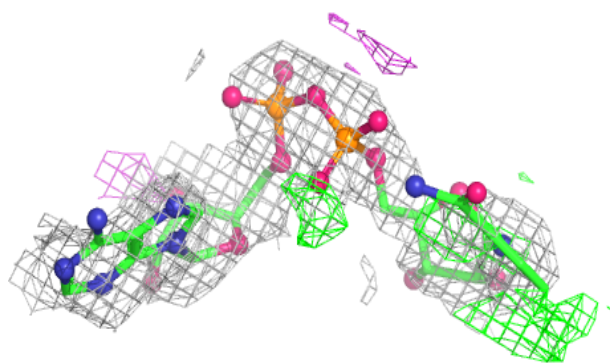
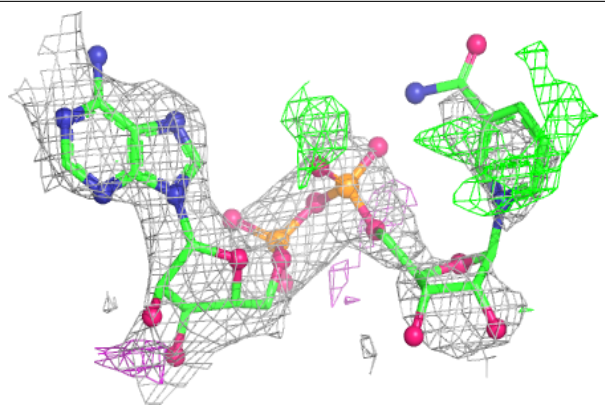
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	MG	D	2004	1/1	0.99	0.12	15,15,15,15	0
9	ZN	D	2002	1/1	1.00	0.03	40,40,40,40	0
9	ZN	N	2001	1/1	1.00	0.02	7,7,7,7	0
9	ZN	D	2001	1/1	1.00	0.02	5,5,5,5	0

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.



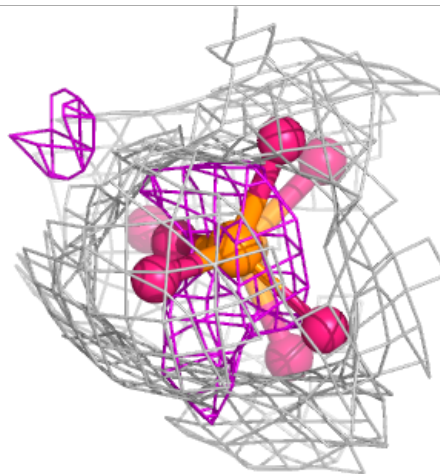
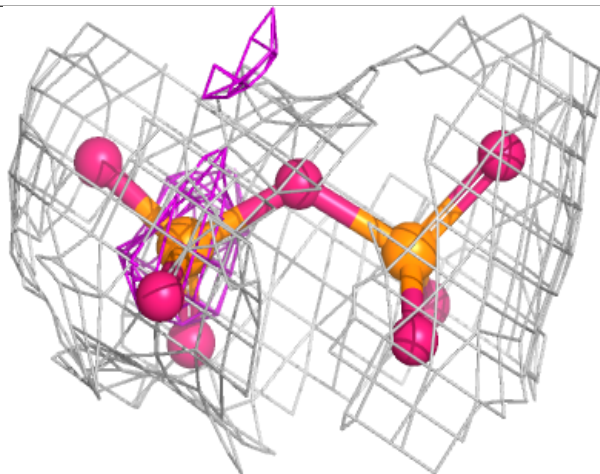
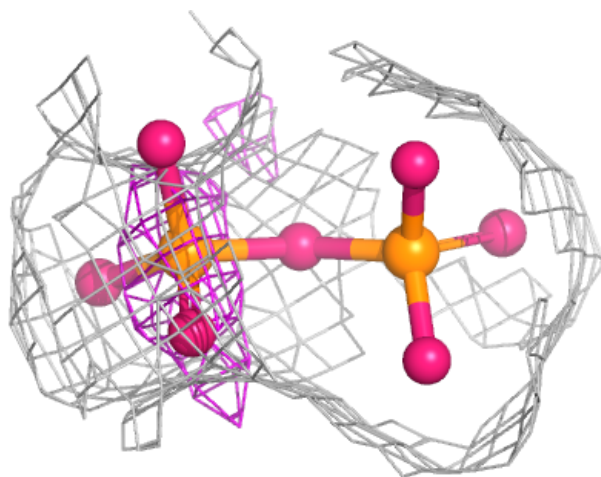
Electron density around NAD G 101:

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



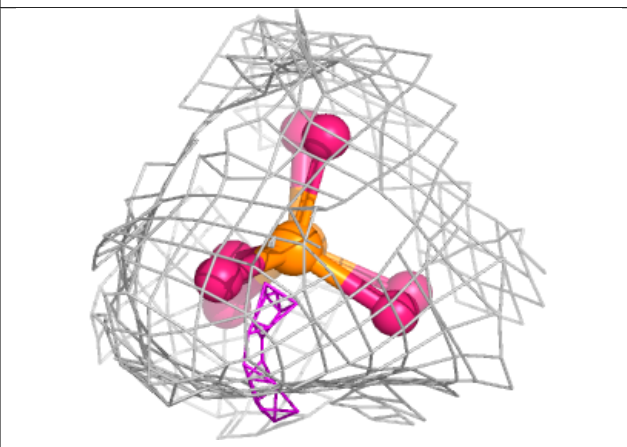
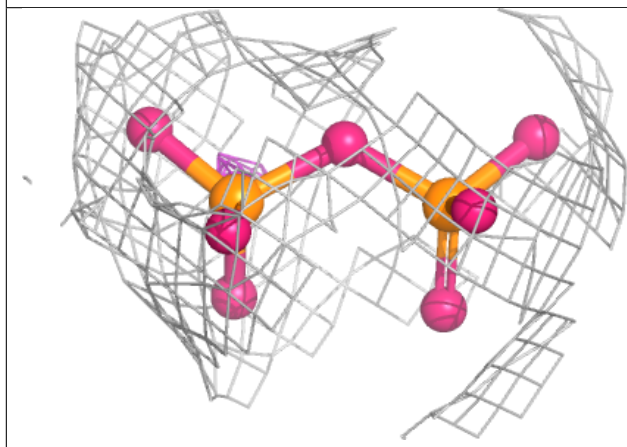
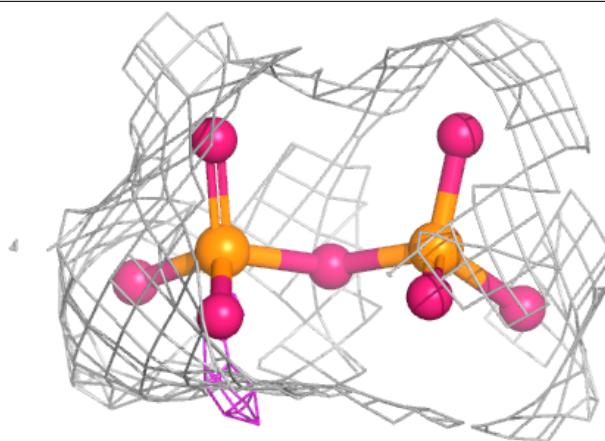
Electron density around CTP M 1201:

$2mF_o-DF_c$ (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.