



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:35 AM UTC

PDB ID : 5X22 / pdb_00005x22
Title : Crystal structure of Thermus thermophilus transcription initiation complex with GpA and CMPcPP
Authors : Zhang, Y.; Ebright, R.
Deposited on : 2017-01-29
Resolution : 3.35 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

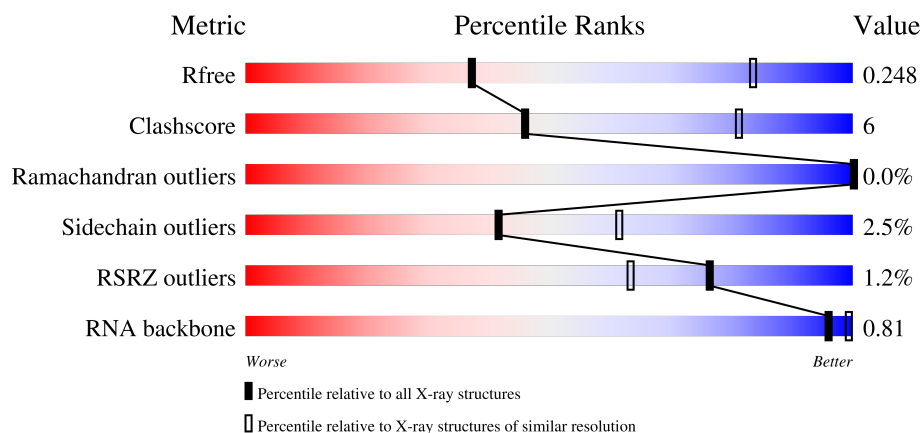
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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	1099 (3.40-3.32)
Clashscore	190562	1116 (3.40-3.32)
Ramachandran outliers	187476	1101 (3.40-3.32)
Sidechain outliers	187428	1101 (3.40-3.32)
RSRZ outliers	180081	1099 (3.40-3.32)
RNA backbone	3983	1110 (3.72-3.00)

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	

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Mol	Chain	Length	Quality of chain
2	C	1119	
2	M	1119	
3	D	1524	
3	N	1524	
4	E	99	
4	O	99	
5	F	443	
5	P	443	
6	G	21	
6	Q	21	
7	H	27	
7	R	27	
8	I	2	
8	S	2	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 56863 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	227	Total	C	N	O	S	0	0	0
			1789	1143	310	334	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	0	0
			8774	5550	1565	1635	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1438	Total	C	N	O	S	0	0	0
			11299	7157	2001	2106	35			
3	N	1500	Total	C	N	O	S	0	0	0
			11834	7499	2086	2213	36			

- 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	327	Total	C	N	O	S	0	0	0
			2649	1671	479	495	4			
5	P	346	Total	C	N	O	S	0	0	0
			2807	1770	509	524	4			

There are 40 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
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
P	-6	LEU	-	expression tag	UNP Q72L95

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Chain	Residue	Modelled	Actual	Comment	Reference
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

- Molecule 6 is a DNA chain called promoter DNA template strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	19	Total	C	N	O	P	0	0	0
			386	184	71	113	18			
6	Q	19	Total	C	N	O	P	0	0	0
			386	184	71	113	18			

- Molecule 7 is a DNA chain called promoter DNA nontemplate strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	27	Total	C	N	O	P	0	0	0
			560	266	109	159	26			
7	R	24	Total	C	N	O	P	0	0	0
			495	236	94	142	23			

- Molecule 8 is a RNA chain called RNA (5'-R(*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	2	Total	C	N	O	P	0	0	0
			42	20	10	11	1			
8	S	2	Total	C	N	O	P	0	0	0
			42	20	10	11	1			

- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	Mg	0	0
			1	1		
9	D	4	Total	Mg	0	1
			5	5		
9	F	1	Total	Mg	0	0
			1	1		
9	L	1	Total	Mg	0	0
			1	1		

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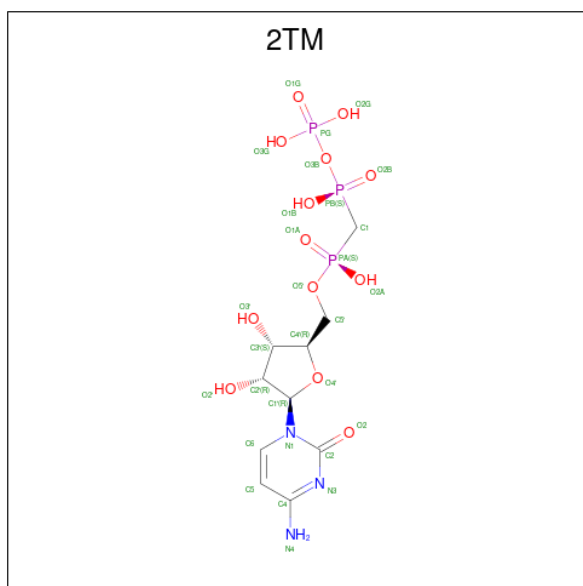
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	N	4	Total	Mg	0	1
			5	5		
9	P	1	Total	Mg	0	0
			1	1		

- Molecule 10 is ZINC ION (CCD ID: ZN) (formula: Zn).

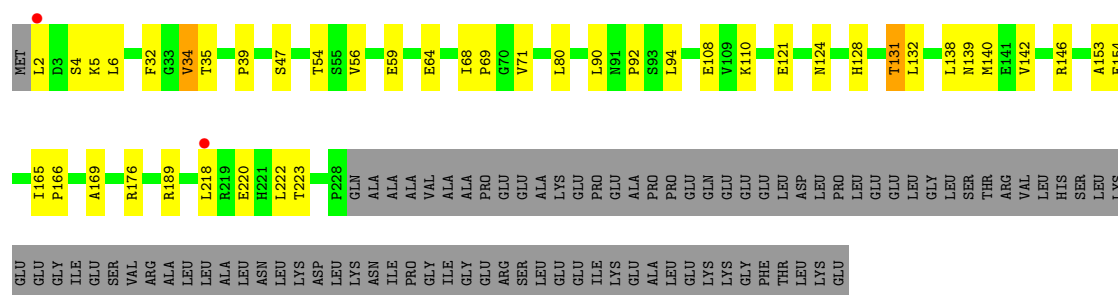
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	D	2	Total	Zn	0	0
			2	2		
10	N	2	Total	Zn	0	0
			2	2		

- Molecule 11 is 5'-O-[(S)-hydroxy{[(S)-hydroxy(phosphonooxy)phosphoryl]methyl}phosphoryl]cytidine (CCD ID: 2TM) (formula: C₁₀H₁₈N₃O₁₃P₃).

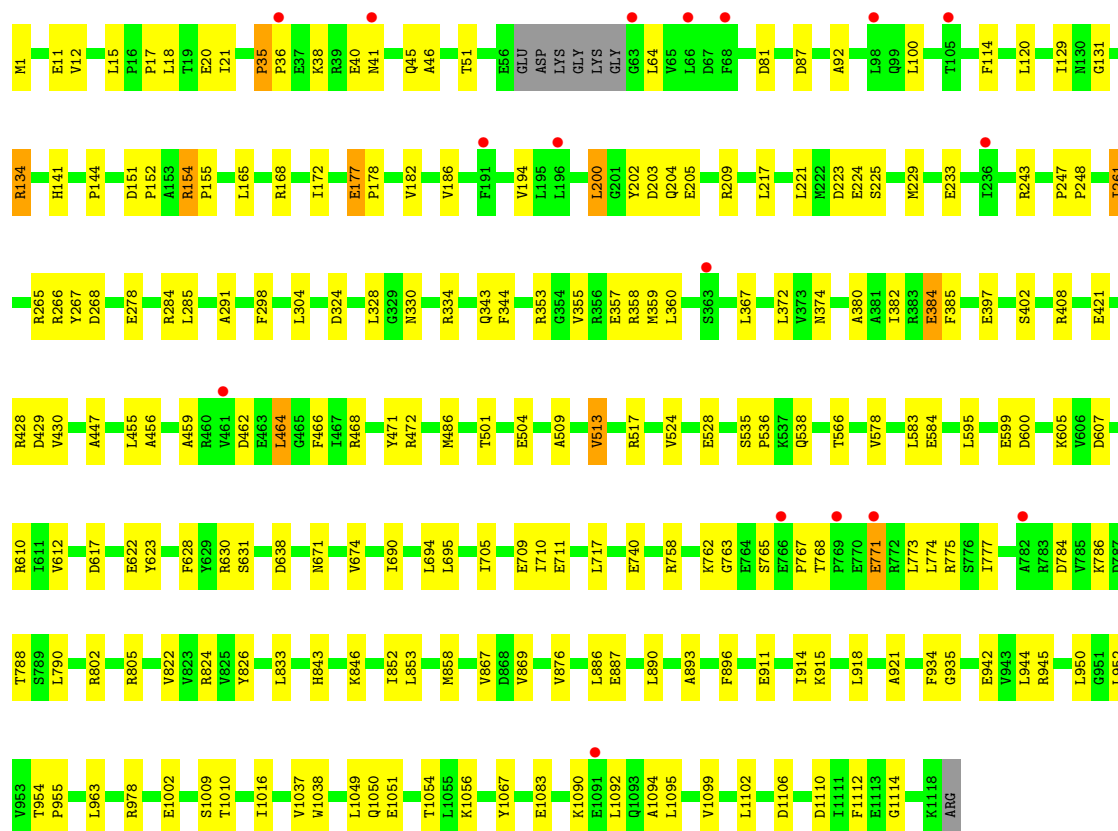


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	D	1	Total	C	N	O	P	0	1
			58	20	6	26	6		
11	N	1	Total	C	N	O	P	0	1
			58	20	6	26	6		

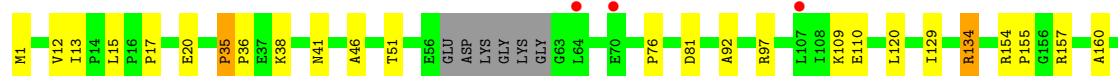
Chain L: %

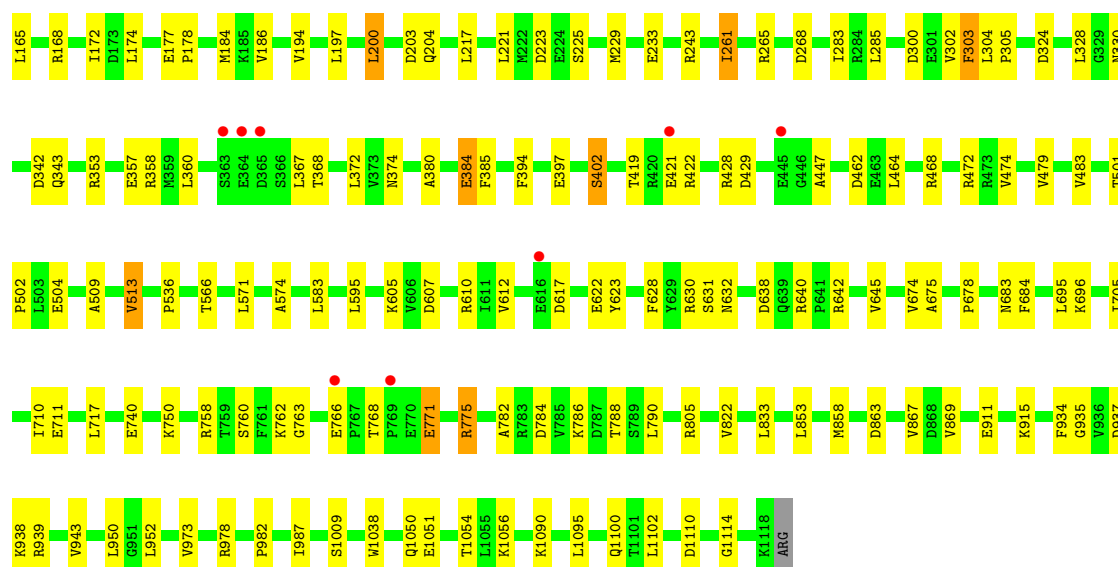


Chain C: 2% 80% 18%

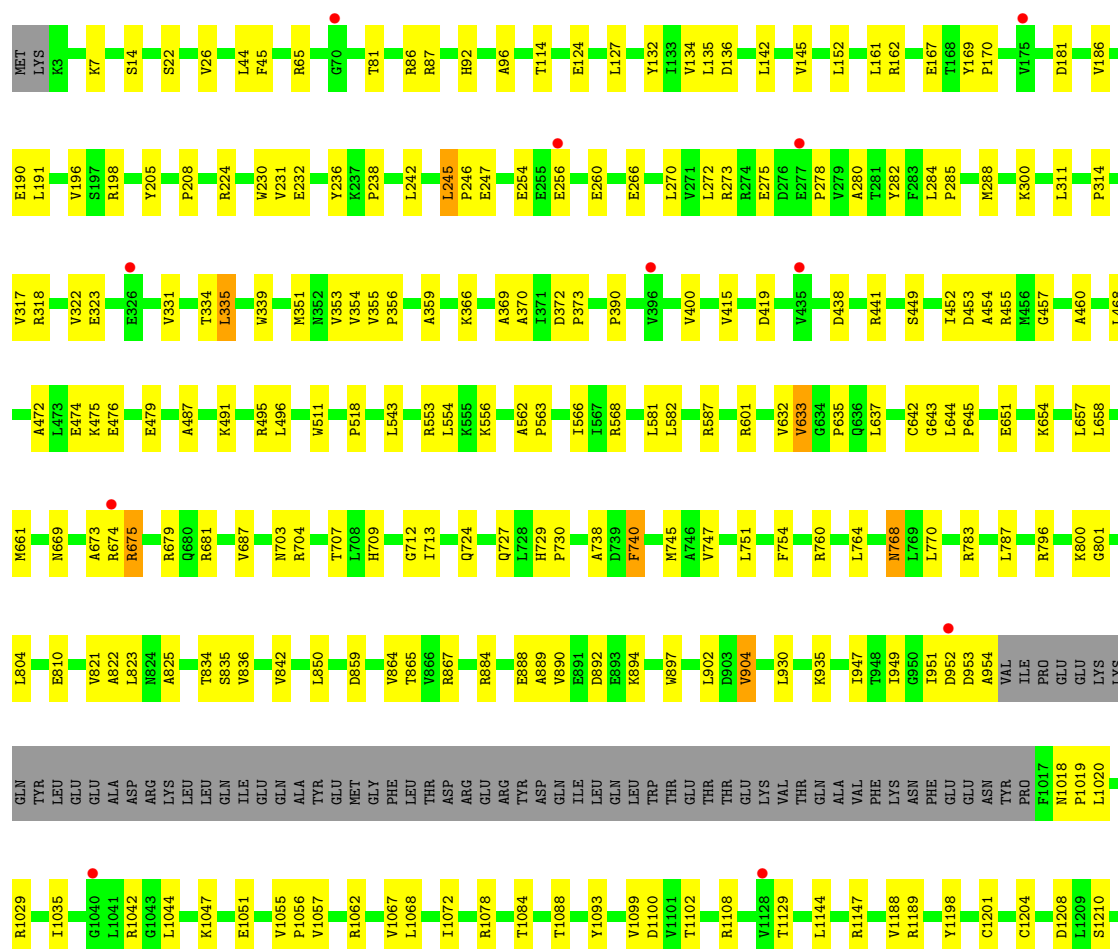
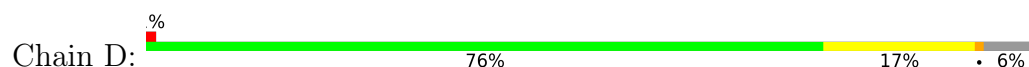


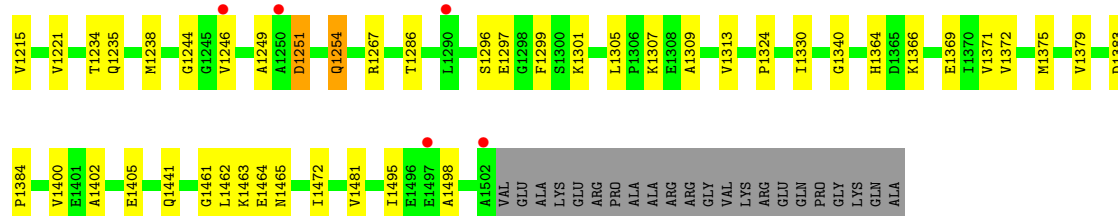
Chain M: %



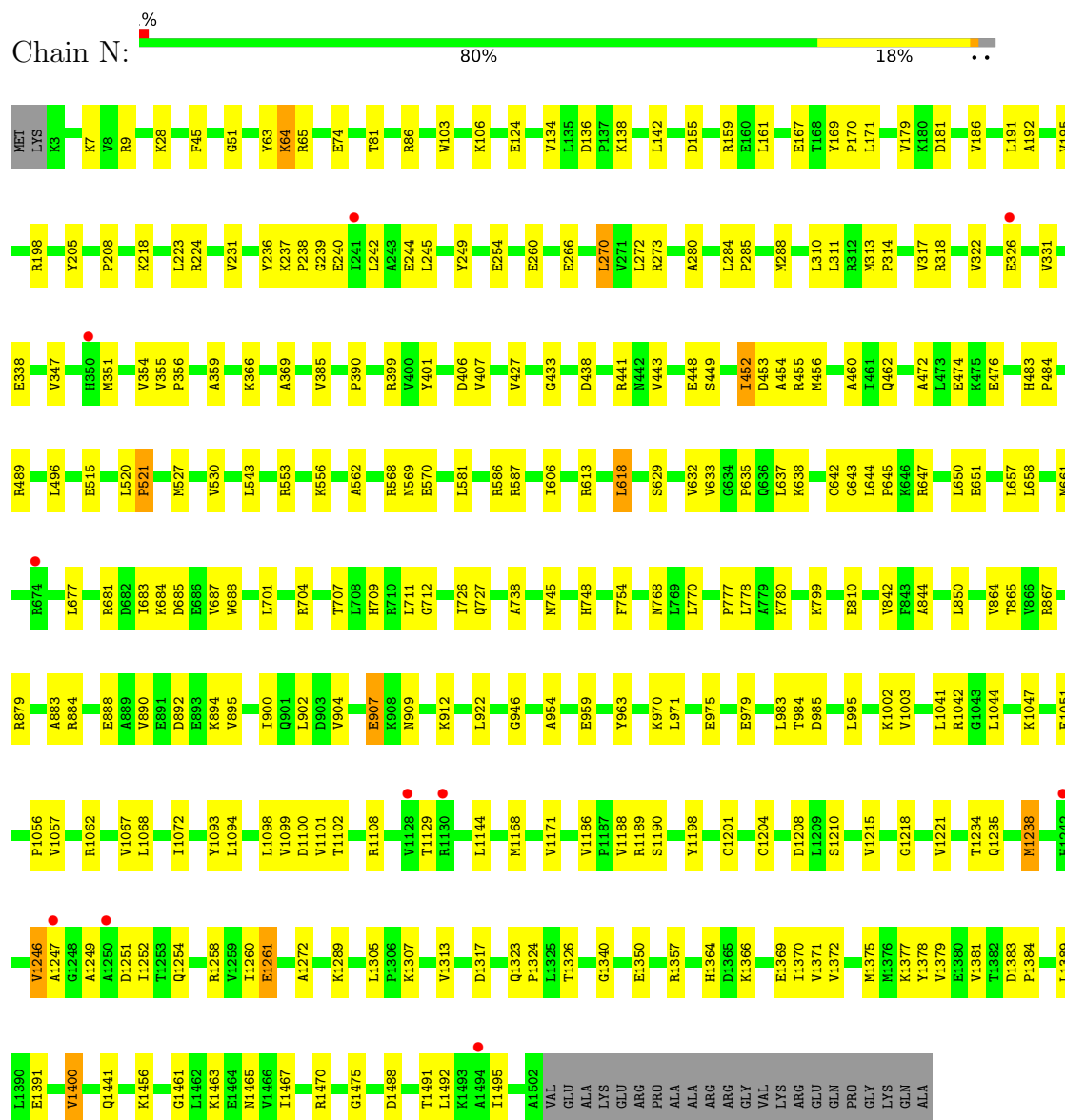


• Molecule 3: DNA-directed RNA polymerase subunit beta'

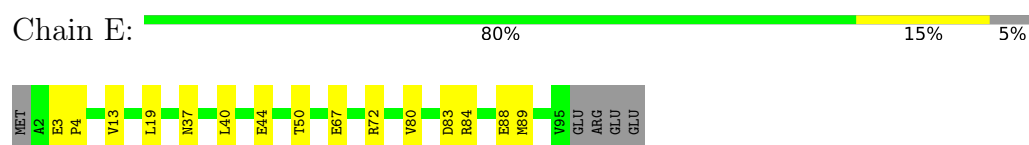




- Molecule 3: DNA-directed RNA polymerase subunit beta'

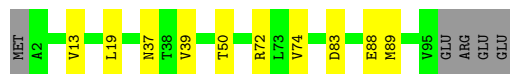


- Molecule 4: DNA-directed RNA polymerase subunit omega



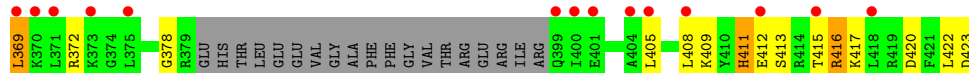
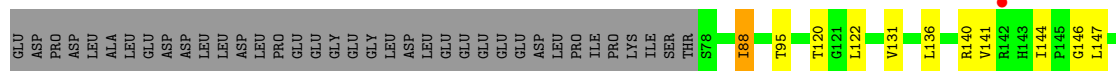
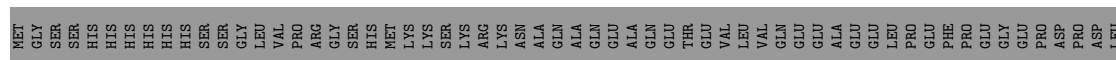
- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain O:  85% 10% 5%



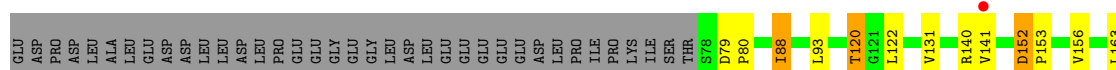
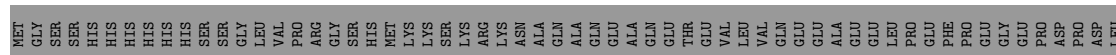
- Molecule 5: RNA polymerase sigma factor SigA

Chain F:  6% 62% 11% 26%



- Molecule 5: RNA polymerase sigma factor SigA

Chain P:  66% 11% 22%

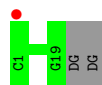
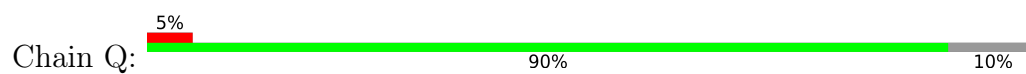


- Molecule 6: promoter DNA template strand

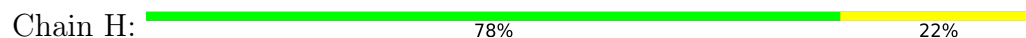
Chain G:  90% 10%



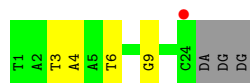
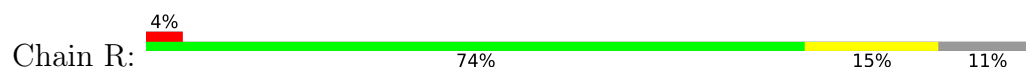
- Molecule 6: promoter DNA template strand



- Molecule 7: promoter DNA nontemplate strand



- Molecule 7: promoter DNA nontemplate strand



- Molecule 8: RNA (5'-R(*GP*A)-3')



- Molecule 8: RNA (5'-R(*GP*A)-3')



There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	186.41 Å 104.32 Å 297.29 Å 90.00° 98.36° 90.00°	Depositor
Resolution (Å)	49.02 – 3.35 49.02 – 3.35	Depositor EDS
% Data completeness (in resolution range)	89.3 (49.02-3.35) 90.6 (49.02-3.35)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 3.33 Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.208 , 0.250 0.207 , 0.248	Depositor DCC
R_{free} test set	7396 reflections (4.45%)	wwPDB-VP
Wilson B-factor (Å ²)	66.5	Xtrriage
Anisotropy	0.043	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 23.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	56863	wwPDB-VP
Average B, all atoms (Å ²)	41.0	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 36.02 % 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 5.3307e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 2TM, 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	0.28	0/1841	0.78	2/2504 (0.1%)
1	B	0.30	0/1790	0.80	1/2435 (0.0%)
1	K	0.28	0/1841	0.79	5/2504 (0.2%)
1	L	0.30	0/1821	0.80	1/2476 (0.0%)
2	C	0.29	0/8941	0.76	4/12092 (0.0%)
2	M	0.29	0/8941	0.76	3/12092 (0.0%)
3	D	0.30	0/11496	0.78	11/15543 (0.1%)
3	N	0.30	0/12043	0.78	13/16284 (0.1%)
4	E	0.26	0/772	0.71	0/1040
4	O	0.28	0/772	0.72	0/1040
5	F	0.29	0/2690	0.74	0/3618
5	P	0.28	0/2852	0.72	0/3837
6	G	0.09	0/432	0.48	0/665
6	Q	0.10	0/432	0.48	0/665
7	H	0.10	0/630	0.54	0/973
7	R	0.10	0/556	0.56	0/858
8	I	0.07	0/47	0.19	0/72
8	S	0.05	0/47	0.14	0/72
All	All	0.29	0/57944	0.76	40/78770 (0.1%)

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	245	LEU	CA-C-N	7.45	127.12	119.82
3	D	245	LEU	C-N-CA	7.45	127.12	119.82
3	D	1340	GLY	CA-C-N	7.23	126.76	119.24
3	D	1340	GLY	C-N-CA	7.23	126.76	119.24
3	N	1340	GLY	CA-C-N	6.49	126.72	119.32
3	N	1340	GLY	C-N-CA	6.49	126.72	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	799	LYS	N-CA-C	6.08	120.83	113.17
2	M	303	PHE	N-CA-C	5.93	118.23	111.11
2	M	35	PRO	CA-C-N	5.78	126.17	119.47
2	M	35	PRO	C-N-CA	5.78	126.17	119.47
3	N	1186	VAL	N-CA-C	5.67	114.20	107.73
3	D	1267	ARG	CA-C-N	5.64	125.65	119.90
3	D	1267	ARG	C-N-CA	5.64	125.65	119.90
1	L	47	SER	N-CA-C	5.60	120.23	113.17
3	N	28	LYS	CA-C-N	5.57	125.18	119.56
3	N	28	LYS	C-N-CA	5.57	125.18	119.56
3	D	275	GLU	CB-CA-C	-5.56	109.67	117.23
1	B	47	SER	N-CA-C	5.38	119.94	113.17
3	D	1481	VAL	N-CA-C	5.32	118.09	112.83
3	N	64	LYS	N-CA-C	5.30	119.85	113.17
1	A	172	SER	CA-C-N	5.29	124.91	119.56
1	A	172	SER	C-N-CA	5.29	124.91	119.56
1	K	172	SER	CA-C-N	5.27	124.88	119.56
1	K	172	SER	C-N-CA	5.27	124.88	119.56
3	D	783	ARG	CB-CA-C	-5.23	110.11	117.23
2	C	35	PRO	CA-C-N	5.21	125.52	119.47
2	C	35	PRO	C-N-CA	5.21	125.52	119.47
3	N	1313	VAL	N-CA-C	5.15	115.54	108.12
1	K	47	SER	N-CA-C	5.13	119.64	113.17
2	C	154	ARG	CA-C-N	5.12	124.74	119.05
2	C	154	ARG	C-N-CA	5.12	124.74	119.05
3	N	51	GLY	CA-C-N	5.12	125.02	119.85
3	N	51	GLY	C-N-CA	5.12	125.02	119.85
3	N	1238	MET	N-CA-C	5.10	119.14	113.02
1	K	91	ASN	CA-C-N	5.07	125.10	119.32
1	K	91	ASN	C-N-CA	5.07	125.10	119.32
3	N	521	PRO	CA-C-N	5.06	124.85	119.28
3	N	521	PRO	C-N-CA	5.06	124.85	119.28
3	D	740	PHE	N-CA-C	5.05	119.14	112.92
3	D	1313	VAL	N-CA-C	5.05	115.40	108.12

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	18	0
1	B	1758	0	1808	29	0
1	K	1809	0	1863	24	0
1	L	1789	0	1841	26	0
2	C	8774	0	8877	131	0
2	M	8774	0	8877	106	0
3	D	11299	0	11543	151	0
3	N	11834	0	12061	156	0
4	E	758	0	770	9	0
4	O	758	0	770	6	0
5	F	2649	0	2728	37	0
5	P	2807	0	2882	30	0
6	G	386	0	215	0	0
6	Q	386	0	215	0	0
7	H	560	0	305	5	0
7	R	495	0	272	3	0
8	I	42	0	23	1	0
8	S	42	0	23	0	0
9	B	1	0	0	0	0
9	D	5	0	0	0	0
9	F	1	0	0	0	0
9	L	1	0	0	0	0
9	N	5	0	0	0	0
9	P	1	0	0	0	0
10	D	2	0	0	0	0
10	N	2	0	0	0	0
11	D	58	0	28	0	0
11	N	58	0	28	0	0
All	All	56863	0	56992	656	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 6.

All (656) 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)
3:D:1495:ILE:HD13	4:E:80:VAL:HG21	1.69	0.75
2:M:168:ARG:HD3	2:M:268:ASP:HB3	1.70	0.73
2:C:194:VAL:HG22	2:C:221:LEU:HD12	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1108:ARG:NH2	3:D:1198:TYR:O	2.22	0.72
2:C:165:LEU:HB2	2:C:168:ARG:HG3	1.71	0.72
2:C:628:PHE:H	2:C:638:ASP:HB3	1.54	0.70
3:N:1108:ARG:NH2	3:N:1198:TYR:O	2.24	0.70
3:D:415:VAL:HG13	3:D:419:ASP:HB2	1.74	0.70
1:K:180:GLN:NE2	2:M:935:GLY:O	2.25	0.70
3:N:1461:GLY:O	3:N:1465:ASN:ND2	2.23	0.70
3:D:1147:ARG:NH2	3:D:1369:GLU:OE1	2.24	0.70
3:D:800:LYS:HB3	3:D:822:ALA:HB2	1.74	0.69
3:D:1498:ALA:HB1	4:E:84:ARG:HH21	1.57	0.69
3:N:356:PRO:HG2	3:N:359:ALA:HB2	1.73	0.69
2:M:194:VAL:HG22	2:M:221:LEU:HD12	1.75	0.69
2:C:674:VAL:HG12	2:C:869:VAL:HB	1.75	0.68
2:C:168:ARG:HD3	2:C:268:ASP:HB3	1.75	0.68
3:D:124:GLU:OE2	3:D:587:ARG:NH2	2.28	0.67
1:L:176:ARG:NH2	3:N:888:GLU:OE1	2.28	0.66
5:P:365:GLU:HB2	5:P:404:ALA:HB2	1.77	0.66
1:A:55:SER:HB3	1:A:143:ARG:HB3	1.77	0.66
2:C:777:ILE:HG23	5:F:412:GLU:HB2	1.77	0.66
2:C:172:ILE:HG12	2:C:186:VAL:HG22	1.77	0.65
2:M:1110:ASP:OD2	2:M:1114:GLY:N	2.29	0.65
3:D:1047:LYS:HD3	3:D:1051:GLU:HB3	1.78	0.65
3:N:266:GLU:HG3	3:N:314:PRO:HB3	1.79	0.65
2:C:758:ARG:HH21	2:C:788:THR:HB	1.62	0.64
2:C:773:LEU:HD23	5:F:354:LEU:HD13	1.79	0.64
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.80	0.64
1:B:176:ARG:NH2	3:D:888:GLU:OE1	2.31	0.64
3:N:1495:ILE:HG12	4:O:88:GLU:HG3	1.80	0.64
2:C:950:LEU:HB3	2:C:952:LEU:HD13	1.80	0.63
3:N:272:LEU:HB2	3:N:280:ALA:HB3	1.79	0.63
3:D:65:ARG:NH1	5:F:378:GLY:O	2.31	0.63
3:D:232:GLU:OE1	3:N:1289:LYS:NZ	2.32	0.63
2:M:165:LEU:HB2	2:M:168:ARG:HG3	1.78	0.63
2:M:428:ARG:NH2	2:M:447:ALA:O	2.31	0.63
1:K:24:VAL:HG22	1:K:196:THR:HG23	1.81	0.63
2:C:344:PHE:HD2	2:C:382:ILE:HD11	1.62	0.62
3:D:804:LEU:HD12	3:D:821:VAL:HG22	1.80	0.62
2:M:12:VAL:HG21	2:M:472:ARG:HD3	1.82	0.62
3:N:45:PHE:O	3:N:86:ARG:NH2	2.32	0.62
3:N:65:ARG:NH1	5:P:378:GLY:O	2.32	0.62
3:D:474:GLU:HG3	3:D:496:LEU:HD11	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:408:LEU:HA	5:F:411:HIS:HD2	1.63	0.62
2:M:628:PHE:H	2:M:638:ASP:HB3	1.64	0.62
1:L:153:ALA:HB1	1:L:166:PRO:HB2	1.80	0.62
1:B:108:GLU:HG2	1:B:131:THR:HG22	1.82	0.62
1:B:56:VAL:HG22	1:B:142:VAL:HG12	1.81	0.61
3:D:356:PRO:HG2	3:D:359:ALA:HB2	1.82	0.61
2:M:229:MET:HB2	2:M:233:GLU:HB2	1.82	0.61
2:M:950:LEU:HB3	2:M:952:LEU:HD13	1.81	0.61
3:N:1047:LYS:HD3	3:N:1051:GLU:HB3	1.81	0.61
3:D:127:LEU:HA	3:D:457:GLY:HA2	1.82	0.61
3:D:285:PRO:HD2	3:D:288:MET:HE2	1.81	0.61
2:M:853:LEU:HB2	2:M:858:MET:HE1	1.83	0.61
3:N:569:ASN:OD1	5:P:214:GLN:NE2	2.34	0.61
5:F:273:ARG:HG2	5:F:276:ARG:HH12	1.66	0.61
2:C:428:ARG:NH2	2:C:447:ALA:O	2.34	0.60
5:P:188:ILE:HD13	5:P:221:ILE:HG12	1.82	0.60
3:N:326:GLU:HG2	3:N:331:VAL:HG12	1.83	0.60
3:D:703:ASN:HB2	3:D:713:ILE:HG12	1.83	0.60
5:F:131:VAL:HG13	5:F:178:ARG:HD3	1.84	0.60
5:P:397:ILE:HD12	5:P:400:ILE:HD11	1.81	0.60
2:M:353:ARG:NH1	2:M:357:GLU:OE2	2.35	0.60
3:N:1201:CYS:SG	3:N:1204:CYS:HB2	2.42	0.60
2:C:92:ALA:HB2	2:C:120:LEU:HD11	1.82	0.60
2:C:711:GLU:HG2	2:C:822:VAL:HG22	1.83	0.60
2:C:12:VAL:HG21	2:C:472:ARG:HD3	1.83	0.60
2:C:408:ARG:NH1	2:C:456:ALA:O	2.35	0.60
3:N:106:LYS:NZ	3:N:124:GLU:OE1	2.35	0.60
3:N:1003:VAL:HG21	3:N:1041:LEU:HG	1.84	0.60
1:A:6:LEU:HD11	1:A:27:PRO:HG2	1.84	0.60
2:M:51:THR:O	2:M:265:ARG:NH2	2.36	0.59
2:M:462:ASP:HB3	2:M:468:ARG:HD2	1.84	0.59
3:N:970:LYS:HD3	3:N:995:LEU:HD13	1.84	0.59
2:C:501:THR:HG21	2:C:513:VAL:HG23	1.85	0.59
1:L:56:VAL:HG22	1:L:142:VAL:HG12	1.83	0.59
3:N:984:THR:OG1	3:N:985:ASP:N	2.36	0.59
5:P:188:ILE:HG12	5:P:224:VAL:HG21	1.84	0.59
2:C:41:ASN:O	2:C:46:ALA:HB2	2.03	0.59
3:N:657:LEU:HG	3:N:661:MET:HE2	1.83	0.59
3:N:954:ALA:O	3:N:1062:ARG:NH2	2.35	0.58
3:N:455:ARG:HB2	3:N:460:ALA:HB2	1.84	0.58
3:N:1350:GLU:OE2	3:N:1357:ARG:NH1	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:273:ARG:HB3	3:D:278:PRO:HA	1.85	0.58
2:M:17:PRO:HB2	2:M:20:GLU:HB3	1.84	0.58
2:M:630:ARG:HB2	2:M:705:ILE:HB	1.85	0.58
3:D:1461:GLY:O	3:D:1465:ASN:ND2	2.37	0.58
1:K:25:LEU:HD23	1:K:28:LEU:HD11	1.86	0.58
2:C:266:ARG:NH1	7:H:11:DG:O6	2.37	0.58
3:N:356:PRO:HB3	3:N:441:ARG:HA	1.86	0.57
3:D:675:ARG:NH2	5:F:420:ASP:OD1	2.37	0.57
1:K:51:THR:OG1	1:K:87:VAL:O	2.20	0.57
2:M:129:ILE:HB	2:M:134:ARG:HD2	1.86	0.57
2:M:402:SER:HA	2:M:566:THR:HG23	1.86	0.57
1:B:77:GLU:OE1	3:D:867:ARG:NH1	2.37	0.57
2:C:802:ARG:HB2	2:C:826:TYR:HB2	1.86	0.57
3:N:218:LYS:HG2	3:N:338:GLU:HG2	1.86	0.57
2:C:324:ASP:O	2:C:330:ASN:ND2	2.35	0.57
2:C:397:GLU:HG3	2:C:631:SER:HB2	1.86	0.57
2:M:197:LEU:HD12	2:M:221:LEU:HD11	1.87	0.57
2:M:1050:GLN:O	2:M:1054:THR:OG1	2.18	0.57
3:N:677:LEU:HD21	3:N:687:VAL:HG21	1.86	0.57
2:M:172:ILE:HG12	2:M:186:VAL:HG22	1.86	0.57
2:M:324:ASP:O	2:M:330:ASN:ND2	2.33	0.57
3:D:142:LEU:HB2	3:D:161:LEU:HD11	1.87	0.57
2:C:367:LEU:HD13	2:C:372:LEU:HD21	1.87	0.56
3:D:208:PRO:HA	3:D:390:PRO:HA	1.87	0.56
1:L:34:VAL:HG21	2:M:978:ARG:HB3	1.87	0.56
1:A:51:THR:OG1	1:A:87:VAL:O	2.22	0.56
2:C:605:LYS:HB2	2:C:612:VAL:HB	1.87	0.56
3:N:171:LEU:HD12	3:N:390:PRO:HG2	1.88	0.56
3:N:179:VAL:O	3:N:205:TYR:OH	2.22	0.56
3:N:704:ARG:HB2	3:N:745:MET:HE2	1.87	0.56
2:C:768:THR:OG1	2:C:771:GLU:OE1	2.24	0.56
3:N:270:LEU:HD12	3:N:284:LEU:HD11	1.88	0.56
3:D:657:LEU:HG	3:D:661:MET:HE2	1.88	0.56
3:N:707:THR:HG23	3:N:712:GLY:HA3	1.86	0.56
5:P:316:SER:HB3	5:P:319:THR:HG23	1.88	0.56
3:N:1258:ARG:NH1	3:N:1261:GLU:OE2	2.34	0.56
2:M:419:THR:HB	2:M:422:ARG:HG3	1.88	0.56
3:N:1100:ASP:OD1	3:N:1463:LYS:NZ	2.36	0.56
2:C:942:GLU:HG3	2:C:945:ARG:HH21	1.70	0.55
2:M:674:VAL:HG12	2:M:869:VAL:HB	1.89	0.55
2:C:129:ILE:HB	2:C:134:ARG:HD2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:369:LEU:HD21	5:F:408:LEU:HD11	1.88	0.55
1:L:4:SER:OG	1:L:189:ARG:NH1	2.39	0.55
3:N:106:LYS:HE2	3:N:587:ARG:HG3	1.88	0.55
1:A:180:GLN:NE2	2:C:935:GLY:O	2.38	0.55
3:D:707:THR:HG23	3:D:712:GLY:HA3	1.88	0.55
2:M:1100:GLN:HG3	3:N:9:ARG:HH21	1.71	0.55
1:K:176:ARG:NH1	2:M:863:ASP:O	2.40	0.55
3:N:124:GLU:OE2	3:N:587:ARG:NH2	2.39	0.55
2:C:762:LYS:HG2	2:C:786:LYS:HD2	1.88	0.55
3:N:260:GLU:OE1	3:N:273:ARG:NH1	2.40	0.55
2:C:64:LEU:HD13	2:C:100:LEU:HD21	1.89	0.54
2:C:177:GLU:HG3	2:C:178:PRO:HD2	1.89	0.54
3:D:953:ASP:HB3	3:D:1018:ASN:HD21	1.72	0.54
3:N:237:LYS:HB2	3:N:240:GLU:HB2	1.89	0.54
5:P:152:ASP:OD1	5:P:152:ASP:N	2.39	0.54
2:C:402:SER:HA	2:C:566:THR:HG23	1.89	0.54
2:M:160:ALA:HB3	2:M:174:LEU:HB2	1.89	0.54
3:N:684:LYS:O	3:N:687:VAL:HG12	2.08	0.54
3:N:894:LYS:H	3:N:894:LYS:HD2	1.72	0.54
3:N:1044:LEU:HD23	3:N:1056:PRO:HB3	1.88	0.54
3:D:272:LEU:HB2	3:D:280:ALA:HB3	1.90	0.54
1:K:218:LEU:HD23	1:L:222:LEU:HD21	1.90	0.54
3:N:134:VAL:HG12	3:N:454:ALA:HB2	1.88	0.54
2:C:853:LEU:HB2	2:C:858:MET:HE1	1.89	0.54
2:C:1094:ALA:HA	3:D:518:PRO:HB2	1.89	0.54
2:C:1102:LEU:HB2	3:D:7:LYS:HB2	1.90	0.54
3:N:1218:GLY:O	3:N:1475:GLY:N	2.34	0.54
3:D:669:ASN:HD22	5:F:417:LYS:HD2	1.73	0.54
5:F:152:ASP:OD1	5:F:152:ASP:N	2.40	0.54
3:N:474:GLU:HG3	3:N:496:LEU:HD11	1.90	0.54
2:M:501:THR:HG21	2:M:513:VAL:HG23	1.90	0.54
3:D:167:GLU:OE2	3:D:198:ARG:NH1	2.41	0.54
2:C:1092:LEU:HD13	2:C:1099:VAL:HG21	1.90	0.53
3:N:711:LEU:HD22	3:N:778:LEU:HD23	1.91	0.53
3:D:1372:VAL:HA	3:D:1375:MET:HE3	1.90	0.53
3:D:890:VAL:HG23	3:D:892:ASP:H	1.72	0.53
3:N:138:LYS:HB2	3:N:452:ILE:HA	1.90	0.53
4:O:39:VAL:O	4:O:72:ARG:NH1	2.37	0.53
2:C:1110:ASP:OD2	2:C:1114:GLY:N	2.40	0.53
3:D:562:ALA:O	5:F:140:ARG:NH1	2.40	0.53
3:N:236:TYR:HD2	3:N:322:VAL:HG21	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:366:LYS:HD3	3:N:369:ALA:HB2	1.89	0.53
3:N:890:VAL:HG23	3:N:892:ASP:H	1.73	0.53
3:D:1495:ILE:HG12	4:E:88:GLU:HG3	1.90	0.53
1:L:128:HIS:HE1	1:L:131:THR:HG23	1.73	0.53
3:N:1093:TYR:OH	3:N:1441:GLN:OE1	2.16	0.53
1:B:80:LEU:HD21	3:D:842:VAL:HG12	1.91	0.53
2:C:353:ARG:NH1	2:C:357:GLU:OE2	2.42	0.53
3:D:14:SER:HB3	3:D:511:TRP:CE2	2.43	0.53
3:N:244:GLU:HG3	3:N:310:LEU:HG	1.91	0.53
3:D:242:LEU:HB3	3:D:311:LEU:HD12	1.91	0.53
1:L:128:HIS:CE1	1:L:131:THR:HG23	2.44	0.53
3:N:406:ASP:OD1	3:N:407:VAL:N	2.40	0.53
3:N:1094:LEU:HD22	3:N:1260:ILE:HG12	1.91	0.53
3:D:563:PRO:HD2	3:D:566:ILE:HD12	1.92	0.52
3:N:245:LEU:HD23	3:N:249:TYR:HB3	1.91	0.52
2:C:35:PRO:HG2	2:C:38:LYS:HB2	1.92	0.52
2:C:1009:SER:HB3	3:D:651:GLU:O	2.09	0.52
3:D:323:GLU:HB2	3:D:334:THR:HB	1.91	0.52
2:M:177:GLU:HG3	2:M:178:PRO:HD2	1.91	0.52
5:P:93:LEU:HD21	5:P:193:ARG:HD2	1.91	0.52
2:M:768:THR:OG1	2:M:771:GLU:OE1	2.28	0.52
3:N:224:ARG:NE	3:N:254:GLU:OE2	2.38	0.52
3:N:136:ASP:HB3	3:N:453:ASP:HB3	1.92	0.52
2:C:695:LEU:HD11	2:C:852:ILE:HD13	1.92	0.52
3:D:633:VAL:HB	3:D:740:PHE:CZ	2.44	0.52
5:F:193:ARG:HB3	7:H:7:DG:H5"	1.91	0.52
2:M:41:ASN:O	2:M:46:ALA:HB2	2.10	0.52
2:M:154:ARG:HE	2:M:157:ARG:HG3	1.75	0.52
3:N:562:ALA:O	5:P:140:ARG:NH1	2.40	0.52
3:N:1102:THR:HG21	3:N:1371:VAL:HG22	1.91	0.52
3:D:1379:VAL:HG21	3:D:1400:VAL:HG11	1.91	0.51
2:M:1038:TRP:CE2	3:N:1099:VAL:HG11	2.45	0.51
2:C:261:ILE:HG23	2:C:291:ALA:HB3	1.91	0.51
3:D:224:ARG:NE	3:D:254:GLU:OE2	2.27	0.51
3:D:272:LEU:HD22	3:D:282:TYR:HE2	1.74	0.51
2:C:1095:LEU:HD23	3:D:582:LEU:HD22	1.92	0.51
2:M:1009:SER:HB3	3:N:651:GLU:O	2.11	0.51
1:B:128:HIS:CE1	1:B:131:THR:HG23	2.46	0.51
2:C:343:GLN:HG3	2:C:385:PHE:HB2	1.93	0.51
3:D:1020:LEU:HB3	3:D:1035:ILE:HD12	1.93	0.51
2:M:607:ASP:HB2	2:M:610:ARG:NH1	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:408:LEU:HA	5:F:411:HIS:CD2	2.44	0.51
2:C:890:LEU:HD13	2:C:914:ILE:HG12	1.92	0.51
2:C:1038:TRP:CE2	3:D:1099:VAL:HG11	2.45	0.51
3:D:266:GLU:HG3	3:D:314:PRO:HB3	1.93	0.51
3:D:822:ALA:HB3	3:D:825:ALA:HB2	1.93	0.51
5:P:361:LEU:HB3	5:P:365:GLU:HG3	1.93	0.51
3:N:192:ALA:HB3	3:N:195:VAL:HB	1.92	0.50
3:N:314:PRO:HB2	3:N:317:VAL:HG12	1.93	0.50
1:A:185:ARG:HH12	1:A:190:THR:HG22	1.76	0.50
5:P:270:LYS:HG2	5:P:295:MET:HE1	1.92	0.50
3:N:644:LEU:HD12	3:N:645:PRO:HD2	1.92	0.50
2:C:144:PRO:HG2	2:C:165:LEU:HD23	1.93	0.50
2:M:243:ARG:NH2	7:R:9:DG:O6	2.45	0.50
3:N:890:VAL:HB	3:N:922:LEU:HD13	1.92	0.50
3:N:1372:VAL:HA	3:N:1375:MET:HE3	1.93	0.50
3:N:399:ARG:HB3	3:N:401:TYR:CE1	2.47	0.50
5:P:131:VAL:HG13	5:P:178:ARG:HD3	1.94	0.50
3:D:366:LYS:HD3	3:D:369:ALA:HB2	1.93	0.50
3:D:644:LEU:HD12	3:D:645:PRO:HD2	1.94	0.50
2:C:21:ILE:HD12	2:C:455:LEU:HD22	1.94	0.49
2:C:154:ARG:NH1	2:C:178:PRO:HG3	2.27	0.49
2:C:343:GLN:NE2	2:C:384:GLU:OE2	2.45	0.49
3:D:438:ASP:OD1	3:D:441:ARG:NH2	2.44	0.49
3:N:704:ARG:HD2	3:N:738:ALA:HB2	1.93	0.49
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.95	0.49
2:C:202:TYR:HE1	2:C:304:LEU:HD22	1.76	0.49
2:M:750:LYS:HD2	3:N:681:ARG:HE	1.76	0.49
2:C:462:ASP:HB3	2:C:468:ARG:HD2	1.94	0.49
2:M:92:ALA:HB2	2:M:120:LEU:HD11	1.94	0.49
2:M:939:ARG:HG2	2:M:982:PRO:HD3	1.95	0.49
3:N:456:MET:HE1	3:N:568:ARG:NE	2.27	0.49
3:N:907:GLU:OE1	3:N:909:ASN:N	2.44	0.49
1:A:53:VAL:HG22	1:A:144:VAL:HG22	1.93	0.49
1:B:34:VAL:HG21	2:C:978:ARG:HB3	1.95	0.49
2:C:630:ARG:HB2	2:C:705:ILE:HB	1.94	0.49
3:N:1190:SER:OG	3:N:1369:GLU:OE1	2.30	0.49
3:N:1465:ASN:OD1	3:N:1470:ARG:NH1	2.46	0.49
2:C:1056:LYS:HE2	3:D:751:LEU:HG	1.95	0.49
2:M:97:ARG:NH1	2:M:110:GLU:OE1	2.32	0.49
2:C:709:GLU:OE2	2:C:824:ARG:NH1	2.46	0.48
3:D:1249:ALA:HB1	3:D:1254:GLN:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:489:ARG:NH1	3:N:1391:GLU:OE2	2.46	0.48
3:D:181:ASP:HB2	3:D:205:TYR:CD1	2.48	0.48
3:D:1068:LEU:O	3:D:1072:ILE:HG12	2.13	0.48
2:M:717:LEU:HD23	2:M:763:GLY:HA2	1.96	0.48
2:M:987:ILE:HD11	3:N:946:GLY:HA2	1.95	0.48
3:D:351:MET:HG2	3:D:370:ALA:HB2	1.94	0.48
1:B:51:THR:OG1	1:B:87:VAL:O	2.28	0.48
2:C:513:VAL:HG13	2:C:524:VAL:HG23	1.95	0.48
3:D:704:ARG:HB2	3:D:745:MET:HG2	1.94	0.48
1:K:56:VAL:HG22	1:K:142:VAL:HG12	1.95	0.48
2:M:76:PRO:HG3	2:M:120:LEU:HD12	1.96	0.48
3:N:63:TYR:OH	3:N:74:GLU:OE2	2.27	0.48
2:C:141:HIS:CE1	2:C:334:ARG:HD2	2.49	0.48
5:F:372:ARG:HH12	5:F:405:LEU:HD13	1.78	0.48
3:N:208:PRO:HA	3:N:390:PRO:HA	1.96	0.48
3:N:864:VAL:HG22	3:N:865:THR:H	1.78	0.48
5:P:120:THR:HB	5:P:122:LEU:HB2	1.95	0.48
3:D:1201:CYS:SG	3:D:1204:CYS:HB2	2.52	0.48
5:F:365:GLU:O	5:F:369:LEU:HB3	2.13	0.48
1:L:90:LEU:HD21	1:L:121:GLU:HB2	1.95	0.48
3:N:629:SER:HB3	3:N:726:ILE:HG13	1.96	0.48
2:C:278:GLU:OE2	2:C:284:ARG:NH2	2.47	0.48
2:C:1067:TYR:OH	3:D:674:ARG:NH1	2.47	0.48
3:D:26:VAL:HG11	3:D:44:LEU:HD23	1.94	0.48
3:D:1324:PRO:HG3	3:D:1330:ILE:HD11	1.95	0.48
2:M:943:VAL:HG11	2:M:973:VAL:HG22	1.96	0.48
3:N:658:LEU:HA	3:N:661:MET:HE3	1.96	0.48
1:B:26:GLU:HB3	1:B:194:LYS:HG3	1.96	0.48
3:D:114:THR:HG23	3:D:495:ARG:HG2	1.96	0.48
3:D:322:VAL:HG22	3:D:335:LEU:HD12	1.96	0.48
3:D:1084:THR:HB	3:D:1238:MET:HA	1.96	0.48
3:D:1244:GLY:O	3:D:1246:VAL:HG23	2.13	0.48
3:D:238:PRO:HG3	3:D:318:ARG:HB2	1.96	0.47
2:M:109:LYS:HG2	2:M:368:THR:HG22	1.95	0.47
3:D:260:GLU:OE1	3:D:273:ARG:NH1	2.41	0.47
2:M:343:GLN:HG3	2:M:385:PHE:HB2	1.97	0.47
2:M:684:PHE:HB3	3:N:633:VAL:HG21	1.95	0.47
2:C:628:PHE:H	2:C:638:ASP:CB	2.25	0.47
1:K:222:LEU:HD21	1:L:218:LEU:HD23	1.95	0.47
3:N:1189:ARG:HB3	3:N:1204:CYS:HA	1.96	0.47
1:A:24:VAL:HG22	1:A:196:THR:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:ILE:HG12	1:A:140:MET:HG2	1.96	0.47
2:C:223:ASP:OD1	2:C:225:SER:OG	2.31	0.47
1:K:20:TYR:OH	1:K:198:ARG:HD2	2.14	0.47
2:M:740:GLU:HB3	2:M:805:ARG:HH12	1.80	0.47
3:N:167:GLU:OE2	3:N:198:ARG:NH1	2.47	0.47
3:N:1144:LEU:HD23	3:N:1144:LEU:HA	1.77	0.47
3:D:1189:ARG:HB3	3:D:1204:CYS:HA	1.95	0.47
5:F:144:ILE:HB	5:F:147:LEU:HD13	1.96	0.47
3:N:543:LEU:HD13	3:N:581:LEU:HA	1.97	0.47
3:N:959:GLU:N	3:N:959:GLU:OE1	2.47	0.47
1:B:90:LEU:HD21	1:B:121:GLU:HB2	1.96	0.47
2:C:430:VAL:HG23	3:D:1078:ARG:HD2	1.96	0.47
2:C:1090:LYS:HE2	2:C:1112:PHE:CZ	2.50	0.47
3:D:654:LYS:O	3:D:658:LEU:HG	2.15	0.47
3:D:661:MET:HE3	3:D:673:ALA:HB1	1.95	0.47
3:D:704:ARG:HD2	3:D:738:ALA:HB2	1.97	0.47
3:D:770:LEU:HB2	3:D:1210:SER:HA	1.97	0.47
3:D:1093:TYR:OH	3:D:1441:GLN:OE1	2.17	0.47
3:D:1100:ASP:OD1	3:D:1463:LYS:NZ	2.41	0.47
2:M:223:ASP:OD1	2:M:225:SER:OG	2.31	0.47
3:N:1068:LEU:O	3:N:1072:ILE:HG12	2.14	0.47
2:C:517:ARG:NH2	2:C:528:GLU:OE2	2.47	0.47
3:D:256:GLU:HG3	3:D:300:LYS:HG3	1.96	0.47
1:K:158:ILE:HD11	1:L:2:LEU:HD13	1.97	0.47
2:M:343:GLN:NE2	2:M:384:GLU:OE2	2.47	0.47
3:N:242:LEU:HB3	3:N:311:LEU:HD12	1.97	0.47
3:D:679:ARG:NH2	3:D:681:ARG:HD2	2.30	0.47
2:M:640:ARG:HE	2:M:642:ARG:HH22	1.62	0.47
2:C:17:PRO:HB2	2:C:20:GLU:HB3	1.97	0.46
3:D:601:ARG:HD3	5:F:318:GLU:HG2	1.97	0.46
3:N:701:LEU:HB2	3:N:748:HIS:HB2	1.97	0.46
1:L:108:GLU:HG2	1:L:131:THR:HG22	1.97	0.46
2:M:15:LEU:HD12	2:M:583:LEU:HD11	1.97	0.46
2:C:595:LEU:HD11	2:C:623:TYR:HB3	1.98	0.46
2:C:843:HIS:NE2	2:C:887:GLU:OE2	2.44	0.46
3:D:935:LYS:HE2	3:D:935:LYS:HB3	1.80	0.46
4:O:13:VAL:HG21	4:O:19:LEU:HB2	1.95	0.46
2:C:717:LEU:CD2	2:C:763:GLY:HA2	2.46	0.46
3:D:132:TYR:OH	3:D:568:ARG:NH1	2.48	0.46
3:D:1234:THR:HG22	3:D:1238:MET:HE2	1.97	0.46
2:M:397:GLU:HG3	2:M:631:SER:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:236:TYR:CD2	3:N:322:VAL:HG21	2.50	0.46
3:N:685:ASP:HA	3:N:688:TRP:HD1	1.80	0.46
2:C:203:ASP:OD2	2:C:204:GLN:N	2.49	0.46
5:F:152:ASP:O	5:F:156:VAL:HG13	2.16	0.46
5:F:153:PRO:HA	5:F:156:VAL:HG22	1.97	0.46
2:M:81:ASP:OD2	2:M:81:ASP:N	2.46	0.46
3:N:1042:ARG:HB3	3:N:1057:VAL:HB	1.96	0.46
1:B:128:HIS:HE1	1:B:131:THR:HG23	1.81	0.46
2:C:380:ALA:O	2:C:384:GLU:HB3	2.14	0.46
3:D:704:ARG:HB2	3:D:745:MET:HE2	1.98	0.46
3:N:155:ASP:OD1	3:N:159:ARG:NH2	2.49	0.46
1:B:112:ARG:HG3	1:B:125:PRO:HB2	1.98	0.46
2:C:612:VAL:HG22	2:C:622:GLU:HG3	1.98	0.46
2:C:774:LEU:HG	5:F:422:LEU:HD13	1.98	0.46
2:C:911:GLU:O	2:C:915:LYS:HG2	2.16	0.46
3:N:1379:VAL:HG21	3:N:1400:VAL:HG11	1.97	0.46
1:A:218:LEU:HD23	1:B:222:LEU:HD21	1.97	0.46
1:K:133:GLU:HG2	1:K:134:GLU:H	1.81	0.46
3:N:438:ASP:OD1	3:N:441:ARG:NH2	2.47	0.46
5:P:193:ARG:HB2	7:R:6:DT:H1'	1.98	0.46
5:F:136:LEU:HD13	5:F:140:ARG:HD2	1.98	0.46
3:N:850:LEU:HD12	3:N:884:ARG:NH2	2.30	0.46
2:C:358:ARG:NH1	2:C:374:ASN:HD22	2.14	0.46
2:C:944:LEU:HD11	2:C:963:LEU:HG	1.98	0.46
2:M:1051:GLU:HB3	2:M:1056:LYS:HE3	1.98	0.46
3:N:9:ARG:HB2	3:N:1456:LYS:HG2	1.98	0.46
3:N:1492:LEU:HD22	4:O:74:VAL:HG21	1.98	0.46
2:C:15:LEU:HD13	2:C:18:LEU:HD21	1.97	0.45
2:C:784:ASP:OD1	2:C:784:ASP:N	2.49	0.45
3:D:864:VAL:HG22	3:D:865:THR:H	1.81	0.45
1:K:50:GLY:HA3	1:K:173:PRO:HD3	1.98	0.45
2:M:394:PHE:CE2	2:M:632:ASN:HB3	2.51	0.45
2:M:710:ILE:HD12	2:M:790:LEU:HB2	1.98	0.45
1:B:110:LYS:HD3	1:B:128:HIS:HA	1.98	0.45
3:D:317:VAL:HG23	3:D:339:TRP:HB3	1.97	0.45
4:O:37:ASN:HD22	4:O:89:MET:HE1	1.80	0.45
1:B:64:GLU:HA	1:B:165:ILE:HD13	1.99	0.45
3:D:230:TRP:NE1	3:D:236:TYR:OH	2.48	0.45
3:D:897:TRP:CH2	3:D:902:LEU:HD22	2.51	0.45
1:K:89:PHE:HD2	1:K:146:ARG:HE	1.65	0.45
2:M:612:VAL:HG22	2:M:622:GLU:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:142:LEU:HB2	3:N:161:LEU:HD11	1.97	0.45
3:N:879:ARG:HD3	3:N:902:LEU:O	2.16	0.45
1:K:198:ARG:HD3	2:M:934:PHE:CZ	2.51	0.45
2:M:367:LEU:HD13	2:M:372:LEU:HD21	1.97	0.45
3:N:1101:VAL:HG13	3:N:1102:THR:HG23	1.98	0.45
5:P:400:ILE:HA	5:P:403:LYS:HG2	1.97	0.45
2:C:462:ASP:OD2	2:C:468:ARG:NH1	2.44	0.45
2:M:1102:LEU:HB2	3:N:7:LYS:HB2	1.99	0.45
2:C:243:ARG:NH2	7:H:9:DG:O6	2.50	0.45
3:N:606:ILE:O	3:N:613:ARG:N	2.48	0.45
5:P:417:LYS:HB3	5:P:418:LEU:HD12	1.99	0.45
3:D:162:ARG:O	3:D:449:SER:HB2	2.17	0.45
3:D:637:LEU:HD13	3:D:642:CYS:HA	1.98	0.45
5:F:188:ILE:HD13	5:F:221:ILE:HG12	1.98	0.45
1:K:101:LEU:HD21	1:K:109:VAL:HG11	1.98	0.45
1:L:94:LEU:O	1:L:146:ARG:NH2	2.50	0.45
3:D:1296:SER:OG	3:D:1297:GLU:N	2.50	0.45
1:K:39:PRO:HG3	1:L:39:PRO:HG3	1.99	0.45
2:M:261:ILE:HD11	2:M:303:PHE:HZ	1.82	0.45
2:M:283:ILE:HD13	2:M:305:PRO:HG2	1.98	0.45
3:N:520:LEU:HD12	3:N:521:PRO:HD2	1.99	0.45
2:C:355:VAL:HG12	2:C:359:MET:HE2	1.99	0.45
3:D:472:ALA:O	3:D:476:GLU:HG2	2.17	0.45
2:M:595:LEU:HD11	2:M:623:TYR:HB3	1.99	0.45
3:N:556:LYS:HD3	5:P:218:GLN:HE22	1.82	0.45
3:D:834:THR:OG1	3:D:835:SER:N	2.50	0.44
1:L:32:PHE:HA	1:L:35:THR:HB	1.99	0.44
2:C:765:SER:O	2:C:767:PRO:HD3	2.17	0.44
2:C:846:LYS:NZ	8:I:2:A:OP1	2.36	0.44
2:C:896:PHE:HB2	2:C:921:ALA:HB1	1.98	0.44
3:D:314:PRO:HB2	3:D:317:VAL:HG12	1.99	0.44
3:D:1383:ASP:HA	3:D:1384:PRO:HD3	1.84	0.44
5:F:295:MET:HA	5:F:295:MET:HE2	1.99	0.44
3:N:106:LYS:O	3:N:586:ARG:NH1	2.50	0.44
1:B:11:PHE:HE1	1:B:23:PHE:HB3	1.82	0.44
3:D:134:VAL:HG12	3:D:454:ALA:HB2	1.99	0.44
5:F:120:THR:HG22	5:F:122:LEU:HD13	1.99	0.44
1:L:124:ASN:OD1	1:L:124:ASN:N	2.50	0.44
5:P:373:LYS:HA	5:P:373:LYS:HD3	1.80	0.44
3:D:190:GLU:HA	3:D:196:VAL:HA	1.98	0.44
3:D:796:ARG:HH12	3:D:859:ASP:HB2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:618:LEU:HG	3:N:1467:ILE:HG23	1.99	0.44
2:C:224:GLU:CD	2:C:224:GLU:H	2.25	0.44
2:C:536:PRO:HB3	3:D:1067:VAL:HG21	2.00	0.44
3:D:1305:LEU:HD13	3:D:1309:ALA:HB3	1.99	0.44
1:K:150:TYR:CD1	2:M:696:LYS:HG2	2.52	0.44
2:M:605:LYS:HB3	2:M:610:ARG:NH1	2.32	0.44
3:N:895:VAL:HG11	3:N:922:LEU:HD21	1.99	0.44
1:K:154:GLU:CD	1:K:154:GLU:H	2.26	0.44
2:M:762:LYS:HG2	2:M:786:LYS:HB3	1.99	0.44
3:N:223:LEU:HD11	3:N:288:MET:HE1	2.00	0.44
3:N:462:GLN:NE2	3:N:515:GLU:OE2	2.44	0.44
1:A:39:PRO:HG3	1:B:39:PRO:HG3	1.99	0.44
2:C:710:ILE:HD12	2:C:790:LEU:HB2	1.99	0.44
2:M:642:ARG:HA	2:M:642:ARG:HD3	1.84	0.44
3:N:483:HIS:CG	3:N:484:PRO:HD2	2.53	0.44
3:N:633:VAL:C	3:N:635:PRO:HD3	2.43	0.44
2:C:1083:GLU:OE2	3:D:87:ARG:NH2	2.51	0.44
5:P:333:ILE:HA	5:P:334:PRO:HD3	1.82	0.44
1:B:73:GLU:HB3	1:B:77:GLU:HB3	2.00	0.44
3:D:889:ALA:HB1	3:D:930:LEU:HA	2.00	0.44
1:K:8:ALA:HA	1:K:9:PRO:HD3	1.89	0.44
2:M:678:PRO:HA	2:M:683:ASN:HD21	1.83	0.44
3:N:1377:LYS:HE3	3:N:1378:TYR:CZ	2.53	0.44
3:N:1381:VAL:HG21	3:N:1389:LEU:HD23	1.99	0.44
1:B:83:LYS:NZ	3:D:842:VAL:O	2.51	0.43
1:B:153:ALA:HA	1:B:156:HIS:NE2	2.33	0.43
2:C:578:VAL:HG23	2:C:671:ASN:CG	2.43	0.43
2:C:740:GLU:HB3	2:C:805:ARG:HH12	1.82	0.43
2:C:1016:ILE:O	3:D:87:ARG:NH1	2.50	0.43
2:M:605:LYS:HB2	2:M:612:VAL:HB	2.00	0.43
3:N:1364:HIS:CE1	3:N:1366:LYS:HG3	2.52	0.43
1:A:64:GLU:HG2	1:A:76:VAL:HG22	2.00	0.43
2:C:87:ASP:HA	2:C:131:GLY:HA3	1.99	0.43
3:D:1462:LEU:HD22	3:D:1472:ILE:HB	2.00	0.43
1:L:80:LEU:HD21	3:N:842:VAL:HG12	1.98	0.43
2:M:617:ASP:OD1	2:M:617:ASP:N	2.50	0.43
2:M:775:ARG:HD3	2:M:782:ALA:HB2	2.00	0.43
3:N:553:ARG:HD2	3:N:570:GLU:OE2	2.18	0.43
1:B:57:TYR:CG	1:B:161:ARG:HD2	2.53	0.43
3:D:372:ASP:HA	3:D:373:PRO:HD3	1.91	0.43
3:N:1249:ALA:HB1	3:N:1254:GLN:CD	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:88:ILE:HD11	5:P:192:LEU:HD13	2.00	0.43
2:C:205:GLU:O	2:C:209:ARG:HG2	2.18	0.43
2:C:328:LEU:HD23	2:C:328:LEU:HA	1.81	0.43
2:C:456:ALA:HB3	2:C:459:ALA:HB2	2.01	0.43
2:C:1051:GLU:HB3	2:C:1056:LYS:HE3	1.99	0.43
3:D:169:TYR:HA	3:D:170:PRO:HD3	1.80	0.43
3:D:1042:ARG:HB3	3:D:1057:VAL:HB	1.99	0.43
5:F:88:ILE:HG23	5:F:193:ARG:HG2	2.00	0.43
2:M:35:PRO:HG2	2:M:38:LYS:HD2	2.00	0.43
3:N:770:LEU:HD23	3:N:777:PRO:HA	2.00	0.43
5:P:153:PRO:HA	5:P:156:VAL:HG22	2.00	0.43
2:C:81:ASP:OD2	2:C:81:ASP:N	2.50	0.43
2:C:200:LEU:HD13	2:C:298:PHE:HB3	2.00	0.43
3:D:1084:THR:O	3:D:1088:THR:OG1	2.34	0.43
7:H:3:DT:H2'	7:H:4:DA:C8	2.54	0.43
3:N:355:VAL:HG11	3:N:385:VAL:HG21	2.00	0.43
3:N:1246:VAL:HG23	3:N:1247:ALA:H	1.82	0.43
3:N:1251:ASP:HB3	3:N:1252:ILE:H	1.55	0.43
1:B:91:ASN:HA	1:B:92:PRO:HD2	1.87	0.43
3:D:633:VAL:O	3:D:635:PRO:HD3	2.18	0.43
1:K:133:GLU:HG3	2:M:645:VAL:HG21	2.00	0.43
2:C:535:SER:O	2:C:538:GLN:HG2	2.18	0.43
2:C:1090:LYS:HD3	2:C:1090:LYS:HA	1.83	0.43
3:D:823:LEU:HA	3:D:836:VAL:HB	2.00	0.43
3:D:1144:LEU:HD23	3:D:1144:LEU:HA	1.77	0.43
3:N:1272:ALA:HA	3:N:1326:THR:HB	2.01	0.43
2:C:695:LEU:HD21	2:C:833:LEU:HB3	2.00	0.43
2:C:858:MET:HG2	2:C:867:VAL:O	2.18	0.43
3:D:1296:SER:HB3	3:D:1299:PHE:HB2	2.00	0.43
1:B:57:TYR:HE1	1:B:163:ASN:HB2	1.83	0.43
2:C:876:VAL:HG11	3:D:949:ILE:HG21	2.00	0.43
3:D:850:LEU:HD12	3:D:884:ARG:NH2	2.34	0.43
5:F:122:LEU:HD21	5:F:159:ILE:HD12	2.00	0.43
2:M:200:LEU:HG	2:M:300:ASP:HB2	2.01	0.43
2:M:766:GLU:OE1	3:N:64:LYS:HB3	2.19	0.43
3:N:181:ASP:HB2	3:N:205:TYR:CD1	2.53	0.43
3:N:780:LYS:HD3	3:N:912:LYS:HD3	2.01	0.43
3:D:455:ARG:HB2	3:D:460:ALA:HB2	2.01	0.43
3:D:543:LEU:HD13	3:D:581:LEU:HA	2.00	0.43
3:N:472:ALA:O	3:N:476:GLU:HG2	2.19	0.43
3:N:883:ALA:HA	3:N:900:ILE:HD13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1168:MET:HE3	3:N:1171:VAL:HB	2.01	0.43
5:P:164:LYS:HA	5:P:171:LYS:HE3	2.01	0.43
3:D:22:SER:HB2	3:D:92:HIS:HB3	2.00	0.42
3:D:270:LEU:HG	3:D:284:LEU:HD11	2.00	0.42
2:M:474:VAL:HG22	2:M:479:VAL:HG22	1.99	0.42
2:M:628:PHE:H	2:M:638:ASP:CB	2.30	0.42
2:M:784:ASP:OD1	2:M:784:ASP:N	2.42	0.42
3:N:242:LEU:HD23	3:N:285:PRO:HG3	2.00	0.42
2:C:247:PRO:HA	2:C:248:PRO:HD3	1.70	0.42
2:C:599:GLU:HG3	2:C:600:ASP:H	1.84	0.42
3:D:954:ALA:HB3	3:D:1062:ARG:NH2	2.35	0.42
2:M:760:SER:O	2:M:786:LYS:HG2	2.19	0.42
3:N:770:LEU:HB2	3:N:1210:SER:HA	2.01	0.42
1:B:64:GLU:HG3	1:B:79:ILE:HD12	2.01	0.42
3:D:487:ALA:O	3:D:491:LYS:HG2	2.19	0.42
3:D:1364:HIS:CE1	3:D:1366:LYS:HG3	2.53	0.42
5:F:405:LEU:HG	5:F:409:LYS:HE3	2.01	0.42
1:K:10:VAL:HG12	1:K:26:GLU:O	2.19	0.42
2:M:504:GLU:HG2	2:M:509:ALA:HB2	2.01	0.42
3:N:637:LEU:HD13	3:N:642:CYS:HA	2.01	0.42
3:N:842:VAL:HG22	3:N:865:THR:HB	2.00	0.42
2:C:954:THR:HA	2:C:955:PRO:HD3	1.86	0.42
2:M:302:VAL:O	2:M:305:PRO:HD2	2.19	0.42
2:M:758:ARG:HH21	2:M:788:THR:HB	1.84	0.42
3:N:1383:ASP:HA	3:N:1384:PRO:HD3	1.85	0.42
4:O:83:ASP:OD1	4:O:83:ASP:N	2.53	0.42
3:D:764:LEU:O	3:D:768:ASN:ND2	2.52	0.42
1:K:89:PHE:HB2	1:K:146:ARG:HH21	1.83	0.42
2:M:13:ILE:HD13	2:M:483:VAL:HG11	2.00	0.42
2:M:911:GLU:O	2:M:915:LYS:HG2	2.19	0.42
2:M:937:ASP:OD1	2:M:938:LYS:N	2.52	0.42
7:R:3:DT:H2'	7:R:4:DA:C8	2.55	0.42
2:C:617:ASP:OD1	2:C:617:ASP:N	2.53	0.42
3:D:246:PRO:HG2	3:D:247:GLU:HG2	2.02	0.42
3:D:633:VAL:HB	3:D:740:PHE:CE2	2.54	0.42
1:L:59:GLU:HB2	1:L:139:ASN:HB3	2.02	0.42
2:M:536:PRO:HB3	3:N:1067:VAL:HG21	2.02	0.42
2:C:168:ARG:O	2:C:267:TYR:HA	2.20	0.42
2:C:229:MET:HB2	2:C:233:GLU:HB2	2.01	0.42
2:C:893:ALA:HB2	2:C:918:LEU:HD23	2.01	0.42
3:D:284:LEU:HD22	3:D:288:MET:HE3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:553:ARG:HD3	5:F:214:GLN:HB3	2.02	0.42
5:F:144:ILE:HG22	5:F:146:GLY:H	1.84	0.42
2:C:114:PHE:CG	5:F:283:GLY:HA2	2.55	0.42
2:C:1037:VAL:HG13	2:C:1049:LEU:HD11	2.00	0.42
3:D:353:VAL:HG12	3:D:355:VAL:H	1.85	0.42
5:F:222:ARG:NH2	5:F:225:GLU:OE1	2.53	0.42
3:N:683:ILE:HG23	3:N:687:VAL:HG11	2.01	0.42
2:C:471:TYR:HB2	2:C:486:MET:HE3	2.01	0.42
2:C:1002:GLU:HA	3:D:724:GLN:OE1	2.19	0.42
3:D:556:LYS:HD3	5:F:218:GLN:HE22	1.85	0.42
4:E:40:LEU:HG	4:E:67:GLU:HG2	2.01	0.42
2:M:1095:LEU:HD13	3:N:103:TRP:CH2	2.55	0.42
5:P:80:PRO:HB2	5:P:210:LEU:HD11	2.01	0.42
1:A:155:LYS:HD2	1:A:155:LYS:HA	1.75	0.42
3:D:96:ALA:HB3	3:D:554:LEU:HD23	2.02	0.42
1:L:68:ILE:HA	1:L:69:PRO:HD3	1.93	0.42
3:N:643:GLY:HA3	3:N:727:GLN:HB2	2.01	0.42
1:A:196:THR:HG21	2:C:934:PHE:HE2	1.85	0.41
3:D:1402:ALA:O	3:D:1405:GLU:HG2	2.20	0.41
1:K:57:TYR:CD1	1:K:161:ARG:HD2	2.55	0.41
2:M:358:ARG:NH1	2:M:374:ASN:HD22	2.18	0.41
3:N:238:PRO:HG3	3:N:318:ARG:HB2	2.01	0.41
3:D:475:LYS:O	3:D:479:GLU:HG2	2.19	0.41
5:F:193:ARG:HB2	7:H:6:DT:H1'	2.02	0.41
1:L:71:VAL:HG22	1:L:132:LEU:HG	2.02	0.41
3:N:527:MET:HE2	3:N:527:MET:HB2	1.96	0.41
2:C:584:GLU:OE2	2:C:584:GLU:N	2.53	0.41
2:M:380:ALA:O	2:M:384:GLU:HB3	2.20	0.41
2:M:853:LEU:HB2	2:M:858:MET:CE	2.49	0.41
3:N:347:VAL:HG13	3:N:351:MET:HB2	2.02	0.41
3:N:433:GLY:HA2	3:N:449:SER:H	1.84	0.41
2:C:15:LEU:HD12	2:C:583:LEU:HD11	2.02	0.41
3:D:245:LEU:HA	3:D:246:PRO:HD2	1.79	0.41
3:D:729:HIS:HA	3:D:730:PRO:HD3	1.95	0.41
3:D:787:LEU:HD21	3:D:947:ILE:HG21	2.01	0.41
2:M:203:ASP:OD2	2:M:204:GLN:N	2.52	0.41
2:M:304:LEU:HB3	2:M:305:PRO:HD3	2.02	0.41
3:N:1491:THR:O	3:N:1495:ILE:HG13	2.20	0.41
1:A:102:LYS:HE3	1:A:102:LYS:HB2	1.81	0.41
1:B:27:PRO:HG3	1:B:186:LEU:HD22	2.00	0.41
2:C:886:LEU:HD21	3:D:951:ILE:HG12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:45:PHE:O	3:D:86:ARG:NH2	2.53	0.41
3:D:556:LYS:HD3	5:F:218:GLN:NE2	2.35	0.41
3:D:1251:ASP:O	3:D:1254:GLN:HG3	2.21	0.41
3:N:650:LEU:HD12	3:N:688:TRP:CH2	2.55	0.41
5:P:210:LEU:HD23	5:P:213:ILE:HD12	2.02	0.41
2:C:51:THR:O	2:C:265:ARG:NH2	2.53	0.41
3:D:468:LEU:HD23	3:D:468:LEU:HA	1.89	0.41
3:D:1102:THR:HG21	3:D:1371:VAL:HG22	2.02	0.41
1:L:92:PRO:O	1:L:146:ARG:NH2	2.54	0.41
1:L:138:LEU:HD21	1:L:140:MET:HE3	2.03	0.41
1:L:220:GLU:O	1:L:223:THR:OG1	2.30	0.41
2:M:35:PRO:HA	2:M:36:PRO:HD3	1.84	0.41
2:M:328:LEU:HD23	2:M:328:LEU:HA	1.79	0.41
3:N:169:TYR:HA	3:N:170:PRO:HD3	1.87	0.41
3:N:1201:CYS:SG	3:N:1204:CYS:CB	3.07	0.41
3:N:1323:GLN:HA	3:N:1324:PRO:HD3	1.97	0.41
1:A:8:ALA:HA	1:A:9:PRO:HD3	1.91	0.41
1:B:153:ALA:HB1	1:B:166:PRO:HB2	2.01	0.41
2:C:1050:GLN:O	2:C:1054:THR:OG1	2.29	0.41
2:C:1106:ASP:OD1	3:D:7:LYS:NZ	2.41	0.41
4:E:44:GLU:OE2	4:E:72:ARG:NH1	2.50	0.41
5:F:212:LEU:HD22	5:F:247:ILE:HG23	2.03	0.41
1:K:59:GLU:HB2	1:K:139:ASN:HB3	2.03	0.41
2:C:464:LEU:HB3	2:C:466:PHE:CD1	2.56	0.41
1:L:64:GLU:HA	1:L:165:ILE:HD13	2.03	0.41
2:M:675:ALA:HB2	2:M:867:VAL:HG11	2.02	0.41
2:M:711:GLU:HG2	2:M:822:VAL:HG22	2.03	0.41
3:N:638:LYS:HD3	3:N:638:LYS:HA	1.87	0.41
3:N:1234:THR:O	3:N:1238:MET:HG2	2.21	0.41
1:B:150:TYR:CE1	1:B:170:VAL:HG22	2.55	0.41
2:C:504:GLU:HG2	2:C:509:ALA:HB2	2.03	0.41
2:C:607:ASP:HB2	2:C:610:ARG:NH1	2.36	0.41
3:D:136:ASP:HB3	3:D:453:ASP:HB3	2.03	0.41
4:E:3:GLU:HA	4:E:4:PRO:HD3	1.94	0.41
1:L:110:LYS:HD3	1:L:128:HIS:HA	2.02	0.41
2:M:154:ARG:HA	2:M:155:PRO:HD3	1.90	0.41
2:M:172:ILE:HD13	2:M:184:MET:HE3	2.03	0.41
2:M:200:LEU:HD13	2:M:200:LEU:HA	1.85	0.41
2:M:717:LEU:CD2	2:M:763:GLY:HA2	2.51	0.41
2:M:1090:LYS:HA	2:M:1090:LYS:HD3	1.80	0.41
3:N:1208:ASP:HB2	3:N:1215:VAL:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:TYR:HE1	1:A:163:ASN:HB2	1.86	0.41
2:C:40:GLU:O	2:C:45:GLN:HG2	2.22	0.41
2:C:151:ASP:HA	2:C:152:PRO:HD2	1.93	0.41
2:C:690:ILE:HB	2:C:694:LEU:HD12	2.02	0.41
3:D:1018:ASN:HA	3:D:1019:PRO:HD3	1.98	0.41
1:L:54:THR:HG22	1:L:169:ALA:HB2	2.03	0.41
3:N:448:GLU:H	3:N:448:GLU:HG2	1.76	0.41
3:N:963:TYR:CE2	3:N:1002:LYS:HD3	2.56	0.41
3:N:975:GLU:O	3:N:979:GLU:HG2	2.19	0.41
2:C:35:PRO:HA	2:C:36:PRO:HD3	1.88	0.40
3:D:760:ARG:O	3:D:764:LEU:HB2	2.21	0.40
3:D:1208:ASP:HB2	3:D:1215:VAL:HA	2.04	0.40
3:D:1301:LYS:HD3	3:D:1301:LYS:HA	1.97	0.40
5:F:188:ILE:HG12	5:F:224:VAL:HG21	2.02	0.40
3:N:239:GLY:H	3:N:313:MET:HB2	1.86	0.40
3:N:844:ALA:O	3:N:867:ARG:HB2	2.21	0.40
3:N:1098:LEU:HD22	3:N:1371:VAL:HG11	2.03	0.40
1:A:172:SER:HA	1:A:173:PRO:HD2	1.92	0.40
2:C:1009:SER:OG	2:C:1010:THR:N	2.54	0.40
3:D:801:GLY:O	3:D:804:LEU:HG	2.22	0.40
4:E:13:VAL:HG21	4:E:19:LEU:HB2	2.03	0.40
4:E:37:ASN:HD22	4:E:89:MET:HE1	1.86	0.40
4:E:83:ASP:OD1	4:E:83:ASP:N	2.54	0.40
2:M:571:LEU:HB2	2:M:574:ALA:HB2	2.03	0.40
3:N:441:ARG:HB2	3:N:443:VAL:HG12	2.03	0.40
5:P:338:LEU:HA	5:P:339:PRO:HD3	1.92	0.40
2:C:154:ARG:HA	2:C:155:PRO:HD3	1.87	0.40
3:D:1044:LEU:HD23	3:D:1056:PRO:HB3	2.03	0.40
5:P:79:ASP:HA	5:P:80:PRO:HD3	1.94	0.40
5:P:285:GLU:HA	5:P:286:PRO:HD3	1.83	0.40
1:B:32:PHE:HA	1:B:35:THR:HB	2.04	0.40
3:N:1366:LYS:O	3:N:1370:ILE:HG12	2.20	0.40
5:P:163:LEU:HD13	5:P:174:LEU:HD13	2.03	0.40
5:P:289:GLU:HG3	5:P:301:ALA:HB2	2.02	0.40
2:C:202:TYR:CE1	2:C:304:LEU:HD22	2.55	0.40
5:F:415:THR:C	5:F:416:ARG:HG2	2.46	0.40
2:M:501:THR:HA	2:M:502:PRO:HD3	1.91	0.40
2:M:695:LEU:HD21	2:M:833:LEU:HB3	2.02	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%)	225 (98%)	4 (2%)	0	100	100
1	B	221/315 (70%)	218 (99%)	3 (1%)	0	100	100
1	K	229/315 (73%)	225 (98%)	4 (2%)	0	100	100
1	L	225/315 (71%)	222 (99%)	3 (1%)	0	100	100
2	C	1108/1119 (99%)	1081 (98%)	27 (2%)	0	100	100
2	M	1108/1119 (99%)	1078 (97%)	30 (3%)	0	100	100
3	D	1434/1524 (94%)	1378 (96%)	55 (4%)	1 (0%)	48	76
3	N	1498/1524 (98%)	1447 (97%)	51 (3%)	0	100	100
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	323/443 (73%)	317 (98%)	6 (2%)	0	100	100
5	P	344/443 (78%)	339 (98%)	5 (2%)	0	100	100
All	All	6903/7630 (90%)	6710 (97%)	192 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	904	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	200/273 (73%)	196 (98%)	4 (2%)	48	65
1	B	196/273 (72%)	190 (97%)	6 (3%)	35	59
1	K	200/273 (73%)	193 (96%)	7 (4%)	32	57
1	L	200/273 (73%)	195 (98%)	5 (2%)	42	61
2	C	936/941 (100%)	919 (98%)	17 (2%)	51	66
2	M	936/941 (100%)	920 (98%)	16 (2%)	53	67
3	D	1203/1279 (94%)	1168 (97%)	35 (3%)	37	60
3	N	1261/1279 (99%)	1230 (98%)	31 (2%)	42	61
4	E	82/88 (93%)	81 (99%)	1 (1%)	63	72
4	O	82/88 (93%)	81 (99%)	1 (1%)	63	72
5	F	285/387 (74%)	271 (95%)	14 (5%)	22	49
5	P	301/387 (78%)	290 (96%)	11 (4%)	30	55
All	All	5882/6482 (91%)	5734 (98%)	148 (2%)	42	61

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	72	LYS
1	A	197	LEU
1	A	205	VAL
1	B	6	LEU
1	B	34	VAL
1	B	72	LYS
1	B	131	THR
1	B	139	ASN
1	B	154	GLU
2	C	1	MET
2	C	11	GLU
2	C	134	ARG
2	C	177	GLU
2	C	182	VAL
2	C	200	LEU
2	C	217	LEU
2	C	261	ILE
2	C	285	LEU
2	C	360	LEU
2	C	384	GLU
2	C	421	GLU

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Mol	Chain	Res	Type
2	C	429	ASP
2	C	464	LEU
2	C	513	VAL
2	C	771	GLU
2	C	775	ARG
3	D	81	THR
3	D	135	LEU
3	D	145	VAL
3	D	152	LEU
3	D	186	VAL
3	D	191	LEU
3	D	231	VAL
3	D	331	VAL
3	D	335	LEU
3	D	354	VAL
3	D	400	VAL
3	D	452	ILE
3	D	632	VAL
3	D	633	VAL
3	D	675	ARG
3	D	687	VAL
3	D	709	HIS
3	D	747	VAL
3	D	754	PHE
3	D	768	ASN
3	D	810	GLU
3	D	894	LYS
3	D	904	VAL
3	D	952	ASP
3	D	1029	ARG
3	D	1055	VAL
3	D	1129	THR
3	D	1188	VAL
3	D	1221	VAL
3	D	1235	GLN
3	D	1251	ASP
3	D	1254	GLN
3	D	1286	THR
3	D	1307	LYS
3	D	1464	GLU
4	E	50	THR
5	F	88	ILE

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Mol	Chain	Res	Type
5	F	95	THR
5	F	141	VAL
5	F	156	VAL
5	F	205	ARG
5	F	310	ILE
5	F	323	ASP
5	F	361	LEU
5	F	367	MET
5	F	369	LEU
5	F	411	HIS
5	F	413	SER
5	F	416	ARG
5	F	423	ASP
1	K	5	LYS
1	K	6	LEU
1	K	59	GLU
1	K	96	THR
1	K	154	GLU
1	K	197	LEU
1	K	205	VAL
1	L	5	LYS
1	L	6	LEU
1	L	34	VAL
1	L	131	THR
1	L	154	GLU
2	M	1	MET
2	M	134	ARG
2	M	200	LEU
2	M	217	LEU
2	M	261	ILE
2	M	285	LEU
2	M	342	ASP
2	M	360	LEU
2	M	384	GLU
2	M	402	SER
2	M	421	GLU
2	M	429	ASP
2	M	464	LEU
2	M	513	VAL
2	M	771	GLU
2	M	775	ARG
3	N	81	THR

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Mol	Chain	Res	Type
3	N	186	VAL
3	N	191	LEU
3	N	231	VAL
3	N	270	LEU
3	N	354	VAL
3	N	427	VAL
3	N	452	ILE
3	N	530	VAL
3	N	618	LEU
3	N	632	VAL
3	N	647	ARG
3	N	709	HIS
3	N	754	PHE
3	N	768	ASN
3	N	810	GLU
3	N	904	VAL
3	N	907	GLU
3	N	971	LEU
3	N	983	LEU
3	N	1129	THR
3	N	1188	VAL
3	N	1221	VAL
3	N	1235	GLN
3	N	1246	VAL
3	N	1261	GLU
3	N	1305	LEU
3	N	1307	LYS
3	N	1317	ASP
3	N	1400	VAL
3	N	1488	ASP
4	O	50	THR
5	P	88	ILE
5	P	120	THR
5	P	141	VAL
5	P	152	ASP
5	P	205	ARG
5	P	295	MET
5	P	310	ILE
5	P	323	ASP
5	P	346	THR
5	P	368	VAL
5	P	380	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	227	ASN
1	B	212	ASN
2	C	343	GLN
2	C	609	ASN
2	C	1019	GLN
3	D	350	HIS
3	D	560	GLN
3	D	669	ASN
3	D	737	ASN
3	D	768	ASN
3	D	855	HIS
3	D	1018	ASN
3	D	1242	HIS
3	D	1254	GLN
3	D	1359	GLN
5	F	218	GLN
5	F	402	ASN
5	F	411	HIS
1	K	227	ASN
1	L	38	ASN
1	L	128	HIS
2	M	343	GLN
2	M	538	GLN
2	M	567	GLN
3	N	388	HIS
3	N	569	ASN
3	N	640	HIS
3	N	703	ASN
3	N	737	ASN
3	N	768	ASN
3	N	1046	GLN
3	N	1242	HIS
3	N	1323	GLN
5	P	175	HIS
5	P	214	GLN
5	P	218	GLN
5	P	402	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	I	1/2 (50%)	0	0
8	S	1/2 (50%)	0	0
All	All	2/4 (50%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 18 are monoatomic - leaving 4 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	2TM	D	2007[A]	9	26,30,30	1.59	6 (23%)	39,47,47	1.15	4 (10%)
11	2TM	N	2007[A]	9	26,30,30	1.87	10 (38%)	39,47,47	1.24	4 (10%)
11	2TM	N	2007[B]	9	26,30,30	1.87	10 (38%)	39,47,47	1.18	4 (10%)
11	2TM	D	2007[B]	9	26,30,30	1.59	6 (23%)	39,47,47	1.22	4 (10%)

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	2TM	D	2007[A]	9	-	3/19/38/38	0/2/2/2
11	2TM	N	2007[A]	9	-	6/19/38/38	0/2/2/2
11	2TM	N	2007[B]	9	-	4/19/38/38	0/2/2/2
11	2TM	D	2007[B]	9	-	4/19/38/38	0/2/2/2

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	2007[A]	2TM	C4-N4	4.10	1.43	1.33
11	N	2007[A]	2TM	C4-N4	4.09	1.43	1.33
11	N	2007[B]	2TM	C4-N4	4.06	1.43	1.33
11	D	2007[B]	2TM	C4-N4	4.06	1.43	1.33
11	N	2007[A]	2TM	PA-O1A	3.05	1.58	1.51
11	N	2007[B]	2TM	PA-O1A	2.99	1.58	1.51
11	N	2007[A]	2TM	C2'-C3'	-2.89	1.45	1.53
11	N	2007[B]	2TM	C2'-C3'	-2.88	1.45	1.53
11	D	2007[B]	2TM	C2'-C3'	-2.86	1.45	1.53
11	D	2007[A]	2TM	C2'-C3'	-2.86	1.45	1.53
11	N	2007[A]	2TM	C3'-C4'	-2.68	1.46	1.53
11	D	2007[B]	2TM	C3'-C4'	-2.66	1.46	1.53
11	N	2007[B]	2TM	C3'-C4'	-2.63	1.46	1.53
11	D	2007[A]	2TM	C3'-C4'	-2.62	1.46	1.53
11	N	2007[A]	2TM	PA-O2A	-2.49	1.50	1.56
11	N	2007[A]	2TM	PB-O2B	2.47	1.57	1.51
11	N	2007[B]	2TM	PA-O2A	-2.45	1.50	1.56
11	N	2007[B]	2TM	PB-O2B	2.43	1.57	1.51
11	N	2007[B]	2TM	PB-O1B	-2.30	1.50	1.56
11	D	2007[A]	2TM	C2-N1	-2.25	1.35	1.40
11	N	2007[B]	2TM	C2-N1	-2.23	1.35	1.40
11	N	2007[A]	2TM	PB-O1B	-2.23	1.50	1.56
11	D	2007[B]	2TM	C2-N1	-2.22	1.35	1.40
11	N	2007[A]	2TM	C2-N1	-2.11	1.35	1.40
11	D	2007[A]	2TM	C2'-C1'	-2.08	1.46	1.53
11	N	2007[B]	2TM	C2'-C1'	-2.06	1.47	1.53
11	D	2007[B]	2TM	C2'-C1'	-2.06	1.47	1.53
11	D	2007[B]	2TM	C6-C5	2.06	1.39	1.35
11	D	2007[A]	2TM	C6-C5	2.05	1.39	1.35
11	N	2007[A]	2TM	C2'-C1'	-2.02	1.47	1.53
11	N	2007[B]	2TM	C6-C5	2.01	1.39	1.35
11	N	2007[A]	2TM	C6-C5	2.01	1.39	1.35

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	N	2007[A]	2TM	PB-O3B-PG	-3.60	119.55	132.45
11	D	2007[B]	2TM	PB-O3B-PG	-3.51	119.86	132.45
11	N	2007[B]	2TM	PB-O3B-PG	-3.42	120.20	132.45
11	D	2007[A]	2TM	PB-O3B-PG	-3.29	120.67	132.45
11	N	2007[A]	2TM	O2-C2-N3	-2.94	117.70	122.33
11	D	2007[B]	2TM	O2-C2-N3	-2.74	118.02	122.33
11	N	2007[B]	2TM	O2-C2-N3	-2.70	118.08	122.33
11	D	2007[B]	2TM	O4'-C4'-C3'	2.69	110.50	105.15
11	N	2007[B]	2TM	O4'-C4'-C3'	2.68	110.47	105.15
11	N	2007[A]	2TM	O4'-C4'-C3'	2.56	110.23	105.15
11	D	2007[A]	2TM	O2-C2-N3	-2.45	118.47	122.33
11	D	2007[A]	2TM	O4'-C4'-C3'	2.36	109.83	105.15
11	D	2007[A]	2TM	C4'-O4'-C1'	-2.34	104.30	109.47
11	N	2007[A]	2TM	C4'-O4'-C1'	-2.21	104.58	109.47
11	N	2007[B]	2TM	C4'-O4'-C1'	-2.20	104.62	109.47
11	D	2007[B]	2TM	C4'-O4'-C1'	-2.16	104.69	109.47

There are no chirality outliers.

All (17) torsion outliers are listed below:

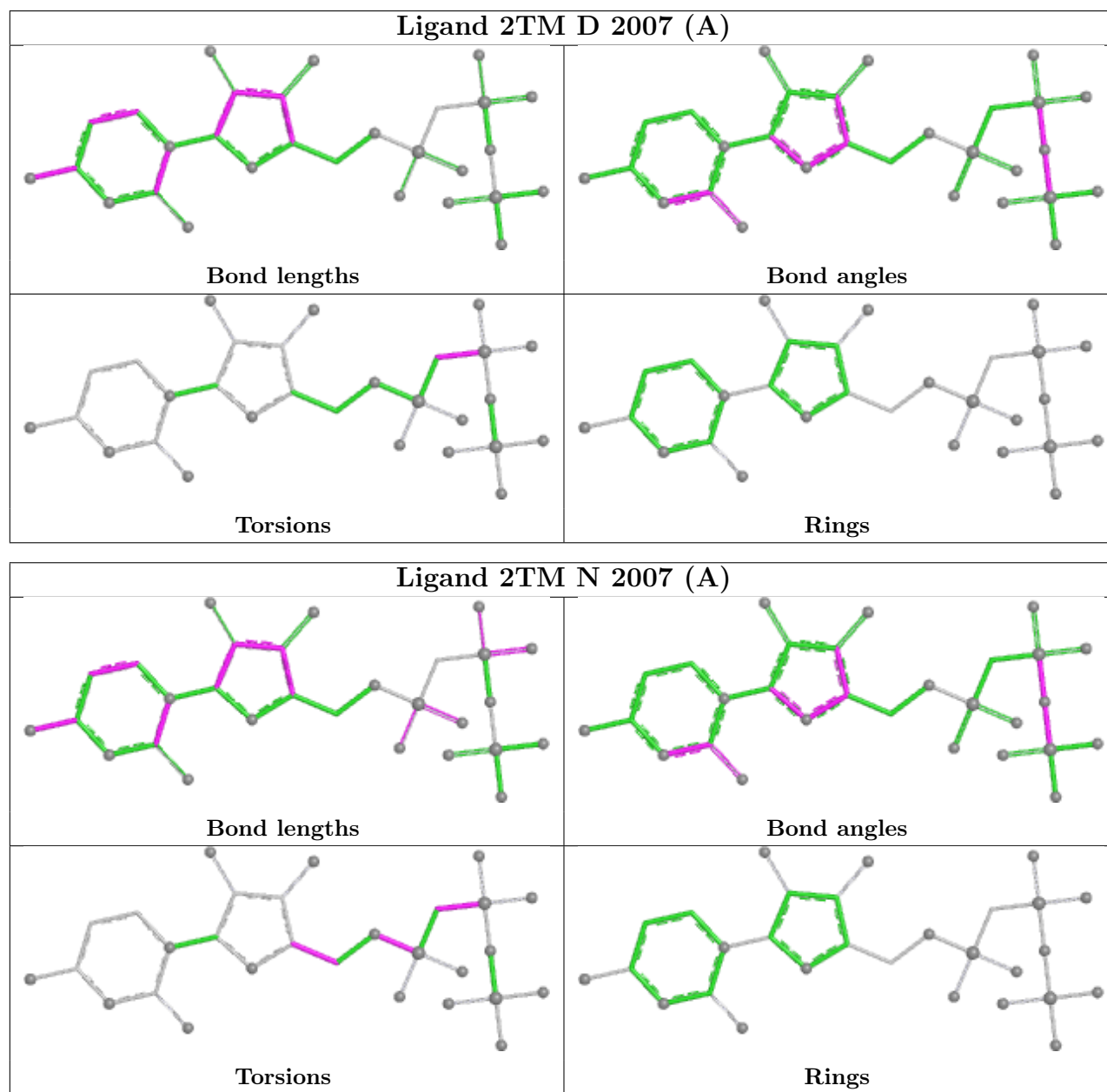
Mol	Chain	Res	Type	Atoms
11	D	2007[A]	2TM	PA-C1-PB-O3B
11	D	2007[A]	2TM	PA-C1-PB-O2B
11	D	2007[B]	2TM	C5'-O5'-PA-O2A
11	D	2007[B]	2TM	O4'-C4'-C5'-O5'
11	N	2007[A]	2TM	C5'-O5'-PA-C1
11	N	2007[A]	2TM	O4'-C4'-C5'-O5'
11	N	2007[A]	2TM	PA-C1-PB-O3B
11	N	2007[A]	2TM	PA-C1-PB-O2B
11	N	2007[B]	2TM	C5'-O5'-PA-O1A
11	D	2007[B]	2TM	C3'-C4'-C5'-O5'
11	N	2007[A]	2TM	C3'-C4'-C5'-O5'
11	N	2007[B]	2TM	O4'-C4'-C5'-O5'
11	N	2007[B]	2TM	C3'-C4'-C5'-O5'
11	D	2007[A]	2TM	PA-C1-PB-O1B
11	N	2007[A]	2TM	PA-C1-PB-O1B
11	D	2007[B]	2TM	PA-C1-PB-O2B
11	N	2007[B]	2TM	C5'-O5'-PA-O2A

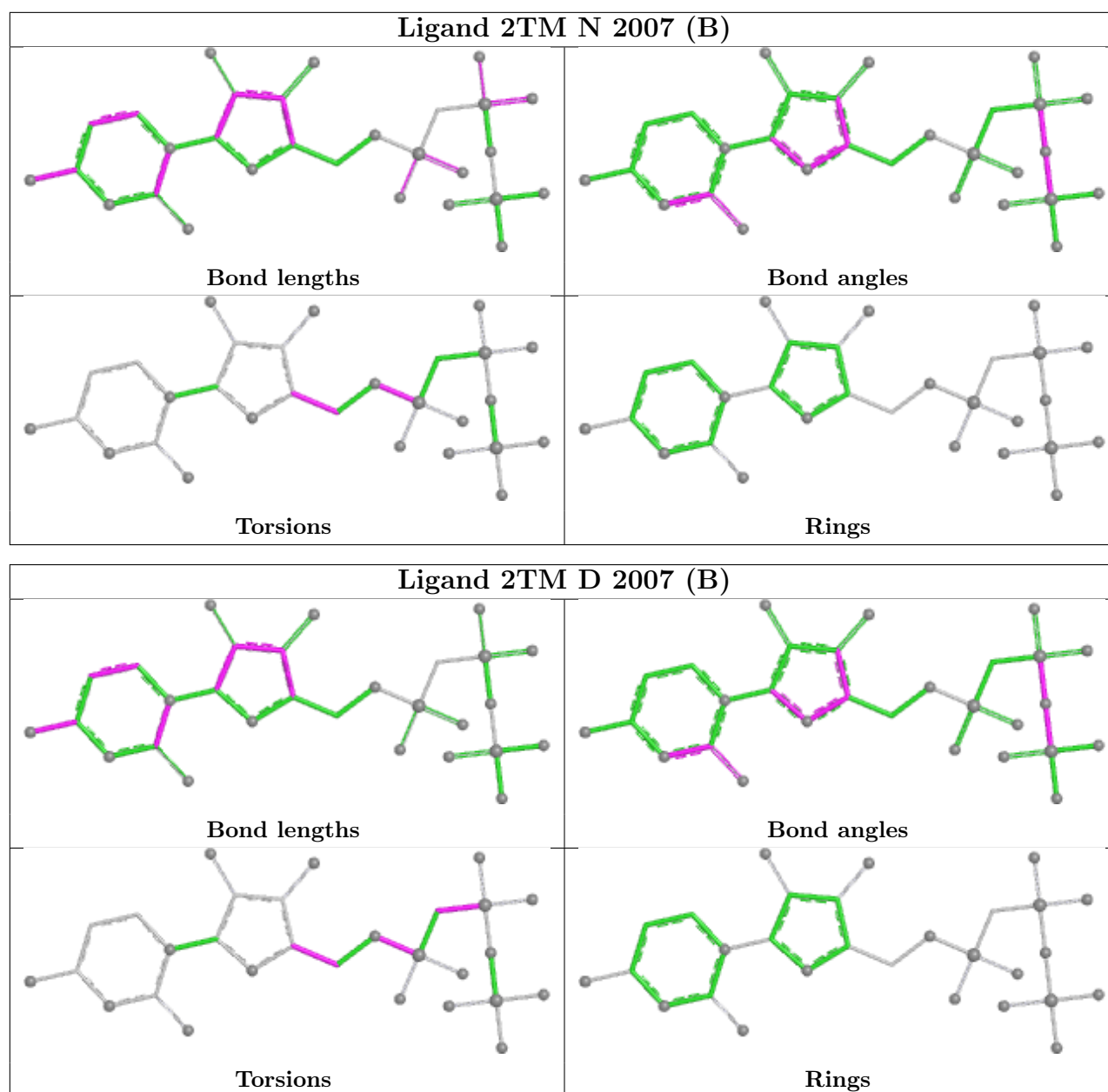
There are no ring outliers.

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%)	-0.02	0 100 100	21, 42, 69, 126	0
1	B	223/315 (70%)	0.02	0 100 100	21, 46, 73, 86	0
1	K	231/315 (73%)	-0.06	1 (0%) 88 81	19, 37, 69, 113	0
1	L	227/315 (72%)	0.02	2 (0%) 81 69	19, 46, 76, 120	0
2	C	1112/1119 (99%)	0.11	17 (1%) 72 57	7, 41, 85, 111	0
2	M	1112/1119 (99%)	-0.17	11 (0%) 79 66	5, 28, 75, 113	0
3	D	1438/1524 (94%)	-0.05	16 (1%) 78 65	5, 33, 88, 133	2 (0%)
3	N	1500/1524 (98%)	-0.09	10 (0%) 84 73	5, 33, 84, 134	2 (0%)
4	E	94/99 (94%)	-0.16	0 100 100	14, 31, 71, 83	0
4	O	94/99 (94%)	-0.01	0 100 100	14, 31, 70, 74	0
5	F	327/443 (73%)	0.42	26 (7%) 18 15	25, 51, 133, 153	0
5	P	346/443 (78%)	-0.05	2 (0%) 85 75	12, 35, 79, 98	0
6	G	19/21 (90%)	0.10	0 100 100	12, 48, 153, 159	0
6	Q	19/21 (90%)	0.17	1 (5%) 32 23	9, 43, 154, 160	0
7	H	27/27 (100%)	0.30	0 100 100	39, 56, 166, 174	0
7	R	24/27 (88%)	0.19	1 (4%) 40 28	27, 51, 113, 130	0
8	I	2/2 (100%)	-0.67	0 100 100	17, 17, 17, 18	0
8	S	2/2 (100%)	-0.95	0 100 100	14, 14, 14, 15	0
All	All	7028/7730 (90%)	-0.02	87 (1%) 76 63	5, 37, 85, 174	4 (0%)

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	F	368	VAL	7.0
5	F	400	ILE	5.7
5	F	367	MET	5.2

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Mol	Chain	Res	Type	RSRZ
5	F	404	ALA	4.6
5	F	408	LEU	4.5
3	D	1497	GLU	4.3
3	N	1250	ALA	4.2
5	F	418	LEU	3.8
5	F	371	LEU	3.8
6	Q	1	DC	3.7
2	C	196	LEU	3.5
5	F	369	LEU	3.5
3	D	326	GLU	3.2
5	F	373	LYS	3.2
3	D	277	GLU	3.1
3	D	435	VAL	3.1
5	F	366	ALA	3.1
5	F	358	LEU	3.1
5	F	364	ARG	3.1
5	F	412	GLU	3.1
3	D	1250	ALA	3.0
5	F	399	GLN	3.0
2	M	365	ASP	2.9
3	D	1502	ALA	2.9
2	C	771	GLU	2.8
2	C	769	PRO	2.8
5	F	375	LEU	2.8
3	D	1040	GLY	2.8
5	F	306	GLU	2.8
3	D	256	GLU	2.7
5	F	357	ALA	2.7
5	F	401	GLU	2.7
3	N	1242	HIS	2.7
5	F	370	LYS	2.7
3	N	1247	ALA	2.7
5	F	142	ARG	2.7
1	L	2	LEU	2.6
2	M	421	GLU	2.6
2	C	461	VAL	2.6
2	C	105	THR	2.6
2	C	782	ALA	2.5
3	N	350	HIS	2.5
3	D	674	ARG	2.5
2	M	445	GLU	2.5
2	C	191	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
3	N	1128	VAL	2.5
5	F	415	THR	2.5
5	F	361	LEU	2.4
2	M	769	PRO	2.4
3	D	70	GLY	2.4
2	M	107	LEU	2.4
2	C	36	PRO	2.4
2	C	1091	GLU	2.4
2	M	616	GLU	2.4
5	F	363	GLU	2.4
2	C	98	LEU	2.3
2	C	68	PHE	2.3
2	C	63	GLY	2.3
2	C	363	SER	2.2
2	M	363	SER	2.2
5	F	359	SER	2.2
3	D	175	VAL	2.2
3	D	396	VAL	2.2
3	D	952	ASP	2.2
3	N	326	GLU	2.2
1	L	218	LEU	2.2
2	C	66	LEU	2.2
3	N	1130	ARG	2.2
2	M	70	GLU	2.2
5	P	141	VAL	2.2
2	M	766	GLU	2.2
5	F	275	ALA	2.2
3	D	1290	LEU	2.1
2	C	766	GLU	2.1
2	C	41	ASN	2.1
5	P	391	GLY	2.1
2	C	236	ILE	2.1
3	N	1494	ALA	2.1
2	M	364	GLU	2.1
7	R	24	DC	2.1
3	D	1246	VAL	2.1
3	N	241	ILE	2.1
3	N	674	ARG	2.1
5	F	405	LEU	2.1
1	K	233	VAL	2.0
3	D	1128	VAL	2.0
2	M	64	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

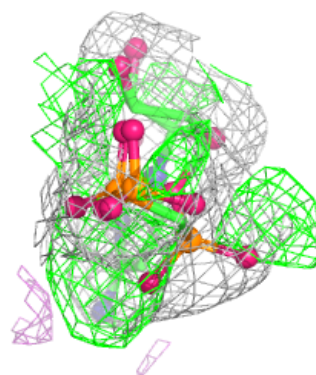
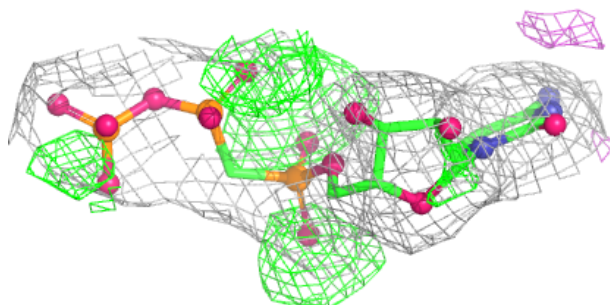
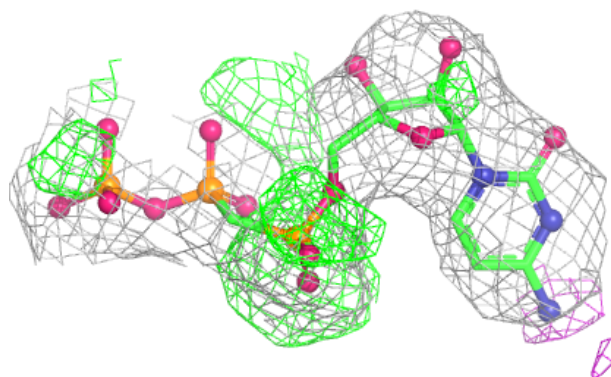
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	MG	N	2006	1/1	0.67	0.11	38,38,38,38	0
9	MG	B	2001	1/1	0.69	0.23	65,65,65,65	0
9	MG	L	2001	1/1	0.72	0.20	54,54,54,54	0
9	MG	D	2006	1/1	0.75	0.08	42,42,42,42	0
9	MG	F	2001	1/1	0.85	0.06	68,68,68,68	0
9	MG	N	2004[A]	1/1	0.88	0.18	25,25,25,25	1
9	MG	N	2004[B]	1/1	0.88	0.18	19,19,19,19	1
9	MG	D	2005	1/1	0.88	0.35	29,29,29,29	0
9	MG	N	2005	1/1	0.89	0.33	25,25,25,25	0
11	2TM	D	2007[A]	29/29	0.89	0.13	14,16,21,22	29
11	2TM	D	2007[B]	29/29	0.89	0.13	14,17,21,22	29
9	MG	P	2001	1/1	0.90	0.07	34,34,34,34	0
11	2TM	N	2007[A]	29/29	0.90	0.13	14,17,25,26	29
11	2TM	N	2007[B]	29/29	0.90	0.13	14,17,25,26	29
9	MG	N	2003	1/1	0.97	0.11	11,11,11,11	0
9	MG	D	2004[B]	1/1	0.98	0.11	18,18,18,18	1
9	MG	D	2003	1/1	0.98	0.04	13,13,13,13	0
9	MG	D	2004[A]	1/1	0.98	0.11	22,22,22,22	1
10	ZN	D	2002	1/1	0.99	0.04	73,73,73,73	0
10	ZN	N	2001	1/1	0.99	0.02	15,15,15,15	0
10	ZN	D	2001	1/1	1.00	0.01	10,10,10,10	0
10	ZN	N	2002	1/1	1.00	0.01	25,25,25,25	0

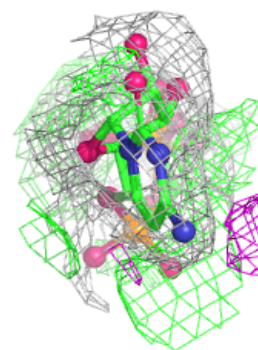
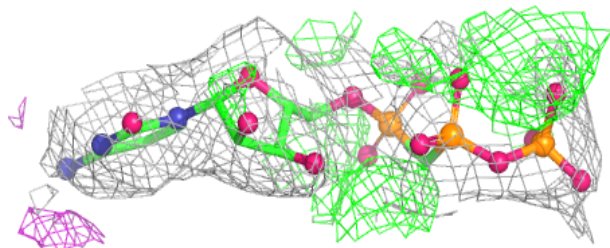
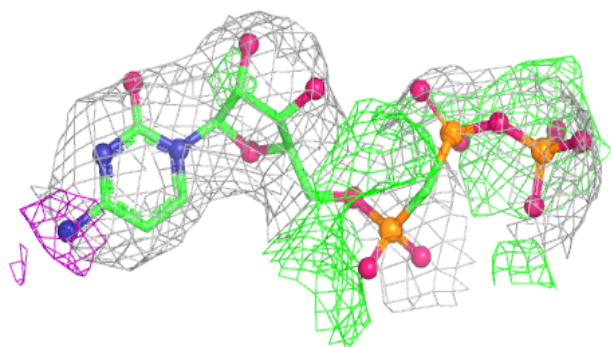
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 2TM D 2007 (A):

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

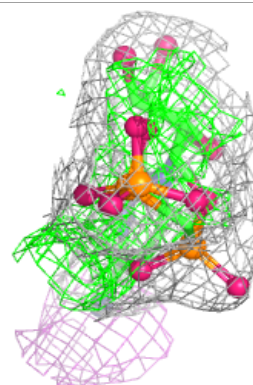
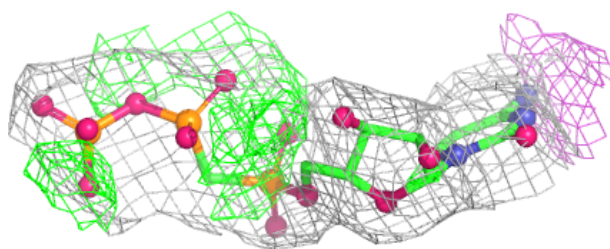
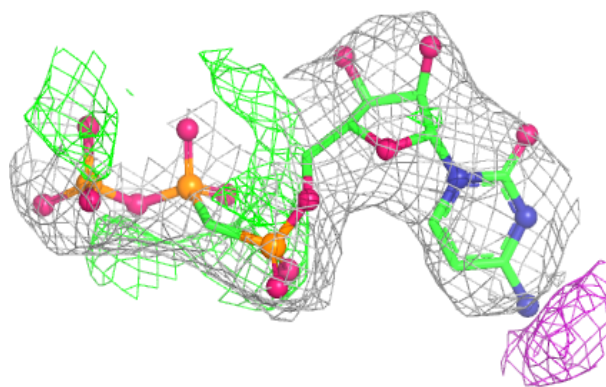
**Electron density around 2TM D 2007 (B):**

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

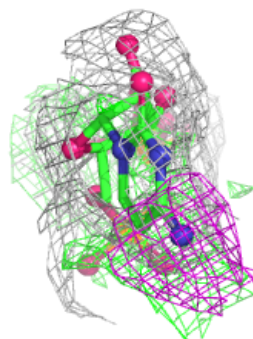
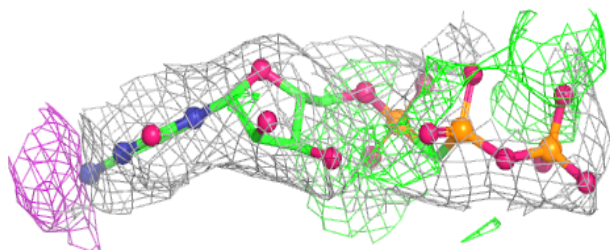
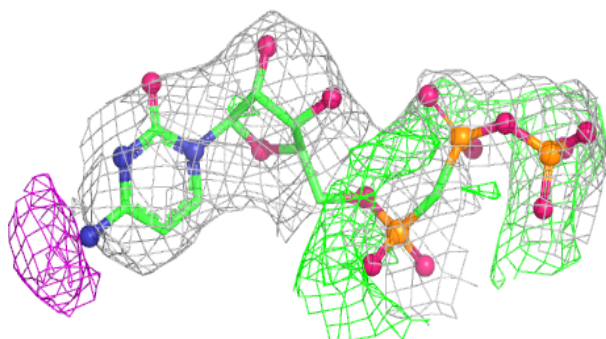


Electron density around 2TM N 2007 (A):

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

**Electron density around 2TM N 2007 (B):**

$2mF_o-DF_c$ (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.