



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:16 PM UTC

PDB ID : 5D4E / pdb_00005d4e
Title : Crystal structure of Thermus thermophilus product complex for transcription initiation with 3'-dephosphate-CoA and CTP
Authors : Zhang, Y.; Ebright, R.H.
Deposited on : 2015-08-07
Resolution : 3.08 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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)
Xtrriage (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

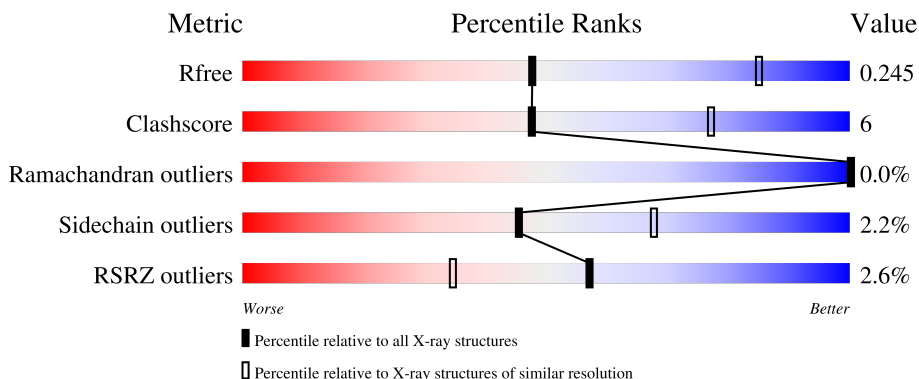
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.08 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2010 (3.10-3.06)
Clashscore	190562	2102 (3.10-3.06)
Ramachandran outliers	187476	1982 (3.10-3.06)
Sidechain outliers	187428	1981 (3.10-3.06)
RSRZ outliers	180081	2010 (3.10-3.06)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	 2% 61% 12% 27%
1	B	315	 60% 11% 29%
1	K	315	 60% 13% 27%
1	L	315	 59% 11% 29%
2	C	1119	 8% 80% 19% 13%

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Mol	Chain	Length	Quality of chain
2	M	1119	<p>% 84% 14% ..</p>
3	D	1524	<p>2% 81% 16% ..</p>
3	N	1524	<p>% 81% 16% .</p>
4	E	99	<p>83% 11% . 5%</p>
4	O	99	<p>81% 14% 5%</p>
5	F	443	<p>7% 62% 15% . 22%</p>
5	P	443	<p>67% 10% 22%</p>
6	H	27	<p>4% 59% 19% 22%</p>
6	S	27	<p>4% 44% 33% 22%</p>
7	G	19	<p>5% 74% 11% 16%</p>
7	R	19	<p>68% 16% 16%</p>

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 57723 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	231	Total	C	N	O	S	0	0	0
			1809	1155	315	337	2			
1	B	223	Total	C	N	O	S	0	0	0
			1758	1124	305	327	2			
1	K	231	Total	C	N	O	S	0	0	0
			1809	1155	315	337	2			
1	L	223	Total	C	N	O	S	0	0	0
			1758	1124	305	327	2			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	1486	Total	C	N	O	S	0	0	0
			11738	7441	2067	2195	35			
3	N	1486	Total	C	N	O	S	0	0	0
			11738	7441	2067	2195	35			

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

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

There are 42 discrepancies between the modelled and reference sequences:

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

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

- Molecule 6 is a DNA chain called DNA (27-MER).

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

- Molecule 7 is a DNA chain called DNA (5'-D(*CP*C*TP*GP*CP*AP*TP*CP*CP*GP*T
P*GP*AP*GP*TP*AP*GP*AP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	16	Total	C	N	O	P	0	0	0
			327	156	62	94	15			
7	R	16	Total	C	N	O	P	0	0	0
			328	157	62	94	15			

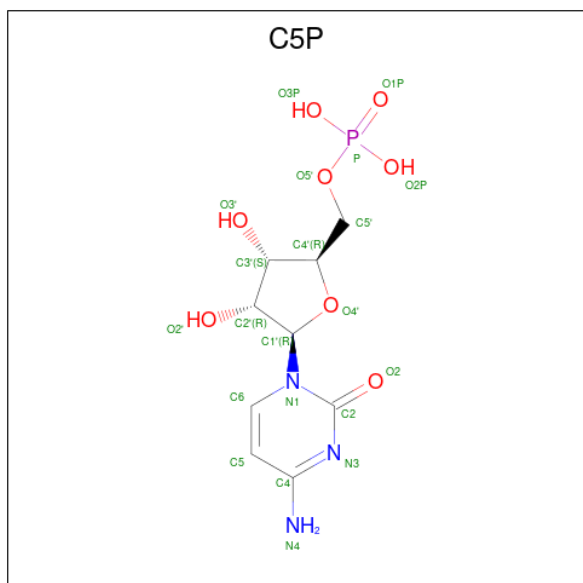
- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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	2	Total	Mg	0	0
			2	2		
8	P	1	Total	Mg	0	0
			1	1		

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

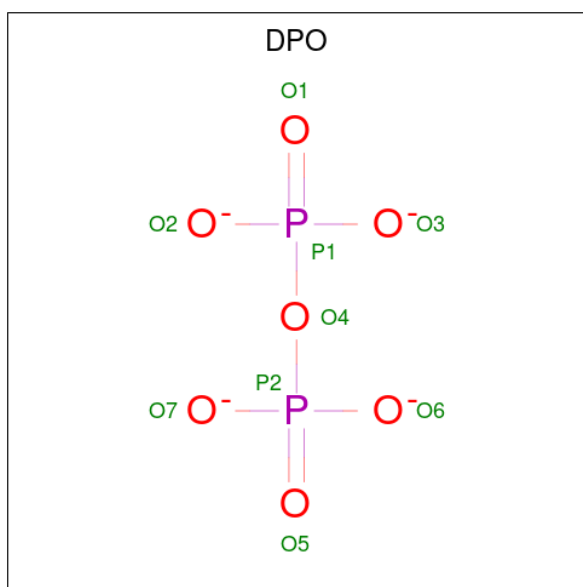
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	D	2	Total	Zn	0	0
			2	2		
9	N	2	Total	Zn	0	0
			2	2		

- Molecule 10 is CYTIDINE-5'-MONOPHOSPHATE (CCD ID: C5P) (formula: C₉H₁₄N₃O₈P).



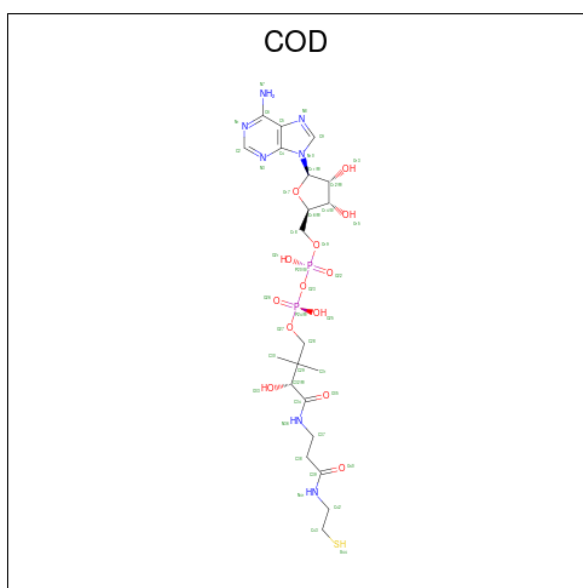
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	D	1	Total	C	N	O	P	0	0
			20	9	3	7	1		
10	N	1	Total	C	N	O	P	0	0
			20	9	3	7	1		

- Molecule 11 is DIPHOSPHATE (CCD ID: DPO) (formula: O₇P₂).



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

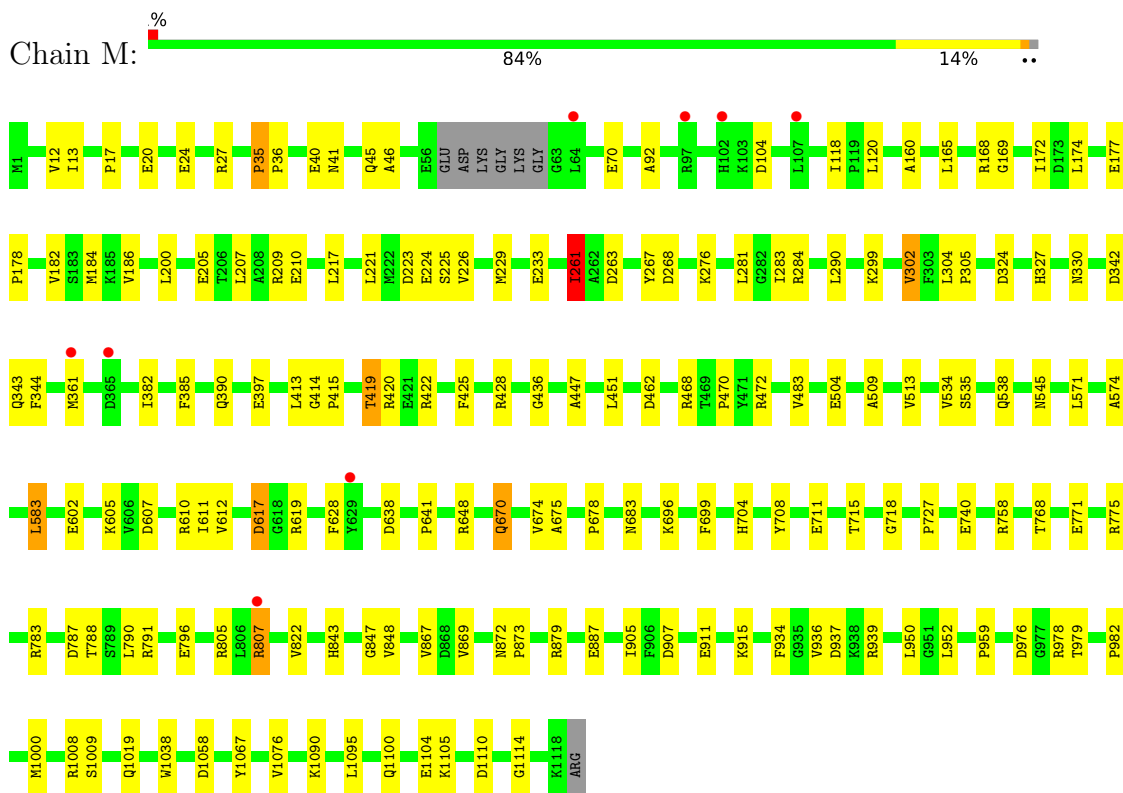
- Molecule 12 is DEPHOSPHO COENZYME A (CCD ID: COD) (formula: C₂₁H₃₅N₇O₁₃P₂S).



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

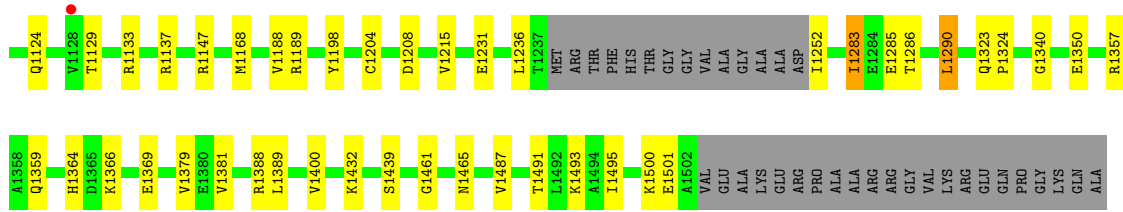
- Molecule 13 is water.

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

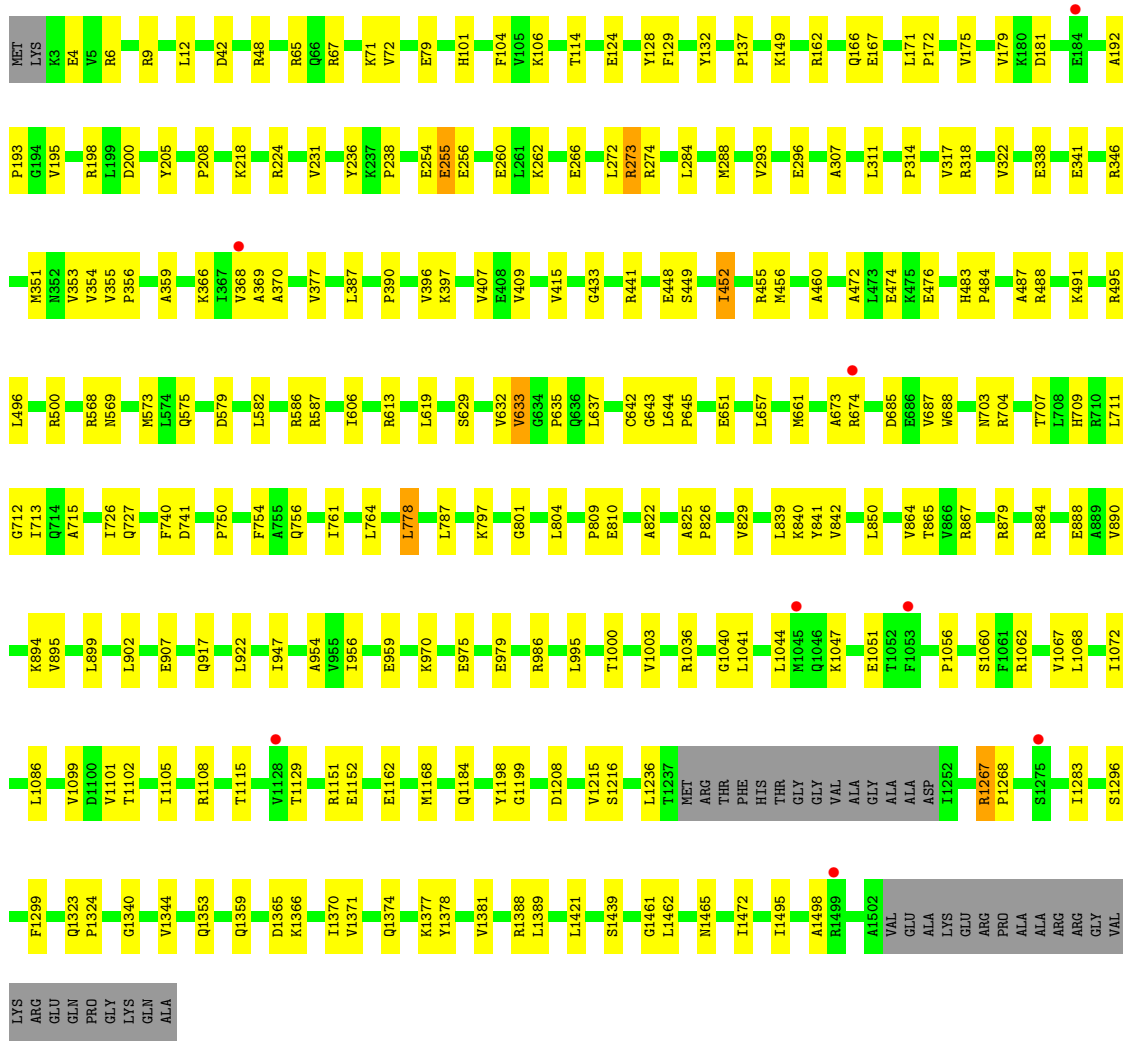
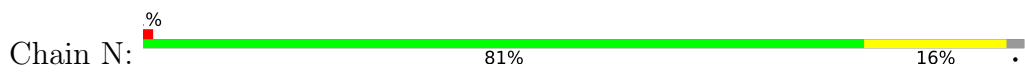


• Molecule 3: DNA-directed RNA polymerase subunit beta'

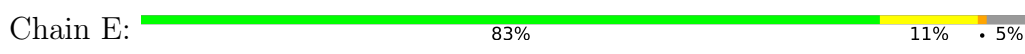




• Molecule 3: DNA-directed RNA polymerase subunit beta'



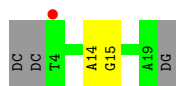
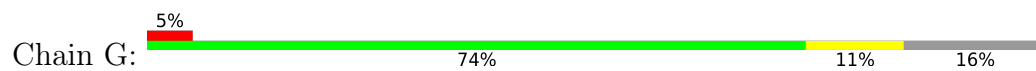
• Molecule 4: DNA-directed RNA polymerase subunit omega



• Molecule 4: DNA-directed RNA polymerase subunit omega



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	185.81Å 103.95Å 297.14Å 90.00° 98.47° 90.00°	Depositor
Resolution (Å)	39.68 – 3.08 39.68 – 3.08	Depositor EDS
% Data completeness (in resolution range)	89.9 (39.68-3.08) 90.1 (39.68-3.08)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 3.06Å)	Xtrriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.210 , 0.246 0.210 , 0.245	Depositor DCC
R_{free} test set	9379 reflections (4.50%)	wwPDB-VP
Wilson B-factor (Å ²)	62.5	Xtrriage
Anisotropy	0.029	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 36.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	57723	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.93 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0674e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, DPO, C5P, COD, MG

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	0.27	0/1841	0.76	2/2504 (0.1%)
1	B	0.35	0/1790	0.81	0/2435
1	K	0.27	0/1841	0.78	2/2504 (0.1%)
1	L	0.35	0/1790	0.82	0/2435
2	C	0.29	0/8941	0.75	3/12092 (0.0%)
2	M	0.30	0/8954	0.75	5/12110 (0.0%)
3	D	0.28	0/11944	0.75	8/16149 (0.0%)
3	N	0.28	0/11944	0.74	3/16149 (0.0%)
4	E	0.25	0/772	0.69	0/1040
4	O	0.26	0/772	0.73	0/1040
5	F	0.28	0/2852	0.76	2/3837 (0.1%)
5	P	0.27	0/2852	0.72	1/3837 (0.0%)
6	H	0.09	0/489	0.49	0/752
6	S	0.10	0/489	0.52	0/752
7	G	0.09	0/367	0.41	0/565
7	R	0.09	0/368	0.46	0/567
All	All	0.28	0/58006	0.74	26/78768 (0.0%)

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	245	LEU	CA-C-N	7.32	127.00	119.82
3	D	245	LEU	C-N-CA	7.32	127.00	119.82
3	D	1231	GLU	CA-C-N	-6.83	114.75	121.65
3	D	1231	GLU	C-N-CA	-6.83	114.75	121.65
3	N	1340	GLY	CA-C-N	6.72	126.23	119.24
3	N	1340	GLY	C-N-CA	6.72	126.23	119.24
3	N	433	GLY	N-CA-C	6.36	119.14	110.69
5	F	394	ARG	CB-CA-C	-6.17	109.47	116.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1340	GLY	CA-C-N	6.16	125.89	119.05
3	D	1340	GLY	C-N-CA	6.16	125.89	119.05
5	F	394	ARG	N-CA-C	6.06	118.32	108.08
2	M	169	GLY	CA-C-N	6.01	125.92	119.85
2	M	169	GLY	C-N-CA	6.01	125.92	119.85
2	C	169	GLY	CA-C-N	5.73	125.64	119.85
2	C	169	GLY	C-N-CA	5.73	125.64	119.85
1	K	172	SER	CA-C-N	5.58	125.20	119.56
1	K	172	SER	C-N-CA	5.58	125.20	119.56
3	D	1018	ASN	CA-C-N	5.48	124.94	119.24
3	D	1018	ASN	C-N-CA	5.48	124.94	119.24
2	C	303	PHE	N-CA-C	5.19	116.62	111.07
5	P	326	ASP	N-CA-C	5.19	116.63	110.97
2	M	35	PRO	CA-C-N	5.12	125.16	119.32
2	M	35	PRO	C-N-CA	5.12	125.16	119.32
1	A	172	SER	CA-C-N	5.06	124.67	119.56
1	A	172	SER	C-N-CA	5.06	124.67	119.56
2	M	261	ILE	N-CA-C	5.00	116.45	111.00

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	1809	0	1863	24	0
1	B	1758	0	1808	24	0
1	K	1809	0	1863	25	0
1	L	1758	0	1808	22	0
2	C	8774	0	8877	129	0
2	M	8783	0	8886	101	0
3	D	11738	0	11971	140	0
3	N	11738	0	11971	137	0
4	E	758	0	770	6	0
4	O	758	0	770	10	0
5	F	2807	0	2882	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	P	2807	0	2882	30	0
6	H	435	0	238	4	0
6	S	435	0	238	6	0
7	G	327	0	179	3	0
7	R	328	0	182	3	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	2	0	0	0	0
8	P	1	0	0	0	0
9	D	2	0	0	0	0
9	N	2	0	0	0	0
10	D	20	0	11	1	0
10	N	20	0	11	3	0
11	D	9	0	0	0	0
11	N	9	0	0	0	0
12	G	28	0	11	0	0
12	R	27	0	11	0	0
13	A	17	0	0	0	0
13	B	10	0	0	0	0
13	C	74	0	0	2	0
13	D	144	0	0	0	0
13	E	8	0	0	0	0
13	F	17	0	0	0	0
13	G	3	0	0	0	0
13	H	6	0	0	0	0
13	K	16	0	0	0	0
13	L	14	0	0	0	0
13	M	178	0	0	3	0
13	N	217	0	0	2	0
13	O	16	0	0	0	0
13	P	41	0	0	0	0
13	R	9	0	0	0	0
13	S	5	0	0	0	0
All	All	57723	0	57232	641	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 (641) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:628:PHE:H	2:C:638:ASP:HB3	1.40	0.86
2:M:168:ARG:HD3	2:M:268:ASP:HB3	1.64	0.79
2:M:165:LEU:HB2	2:M:168:ARG:HG3	1.63	0.78
2:C:802:ARG:HB2	2:C:826:TYR:HB2	1.66	0.75
2:C:165:LEU:HB2	2:C:168:ARG:HG3	1.68	0.74
2:M:628:PHE:H	2:M:638:ASP:HB3	1.51	0.74
2:C:168:ARG:HD3	2:C:268:ASP:HB3	1.69	0.73
2:M:428:ARG:NH2	2:M:447:ALA:O	2.22	0.72
3:N:351:MET:HG2	3:N:370:ALA:HB2	1.72	0.72
2:C:711:GLU:HG2	2:C:822:VAL:HG22	1.73	0.71
3:N:1495:ILE:HD13	4:O:80:VAL:HG21	1.73	0.71
3:N:1495:ILE:HG12	4:O:88:GLU:HG3	1.72	0.70
3:D:1108:ARG:NH2	3:D:1198:TYR:O	2.25	0.69
2:C:28:ARG:HH22	2:C:42:VAL:HG21	1.58	0.69
3:N:1461:GLY:O	3:N:1465:ASN:ND2	2.26	0.68
2:C:674:VAL:HG12	2:C:869:VAL:HB	1.76	0.68
5:F:273:ARG:HG2	5:F:276:ARG:HH12	1.58	0.68
3:N:218:LYS:HG2	3:N:338:GLU:HG2	1.77	0.67
2:C:605:LYS:HB2	2:C:612:VAL:HB	1.75	0.66
3:N:1108:ARG:NH2	3:N:1198:TYR:O	2.28	0.66
3:N:124:GLU:OE2	3:N:587:ARG:NH2	2.29	0.66
3:D:256:GLU:HG3	3:D:300:LYS:HG3	1.79	0.65
3:D:208:PRO:HA	3:D:390:PRO:HA	1.78	0.64
2:C:541:SER:O	2:C:545:ASN:ND2	2.27	0.64
1:K:222:LEU:HD22	1:L:215:VAL:HG23	1.78	0.64
3:D:657:LEU:HG	3:D:661:MET:HE2	1.78	0.64
1:K:106:PRO:HG3	1:K:134:GLU:HG2	1.78	0.64
5:F:392:VAL:HG11	5:F:396:ARG:HD3	1.79	0.64
1:L:176:ARG:NH2	3:N:888:GLU:OE1	2.30	0.64
3:D:415:VAL:HG13	3:D:419:ASP:HB2	1.80	0.64
3:N:167:GLU:OE2	3:N:198:ARG:NH1	2.30	0.64
2:M:24:GLU:OE2	2:M:27:ARG:NH2	2.31	0.64
7:R:18:DG:H2''	7:R:19:DA:H5'	1.80	0.64
2:M:1100:GLN:HG3	3:N:9:ARG:HH21	1.62	0.63
2:M:343:GLN:HG3	2:M:385:PHE:HB2	1.80	0.63
3:N:970:LYS:HD3	3:N:995:LEU:HD13	1.79	0.63
5:F:279:GLN:HB3	5:F:286:PRO:HD3	1.80	0.63
2:M:290:LEU:HD22	2:M:302:VAL:HG11	1.80	0.63
3:N:260:GLU:OE1	3:N:273:ARG:NH1	2.32	0.63
3:D:124:GLU:OE2	3:D:587:ARG:NH2	2.32	0.62
3:D:127:LEU:HA	3:D:457:GLY:HA2	1.81	0.62
2:M:939:ARG:HG2	2:M:982:PRO:HD3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:171:LEU:HD12	3:N:390:PRO:HG2	1.81	0.62
2:C:939:ARG:HG2	2:C:982:PRO:HD3	1.80	0.62
2:C:408:ARG:NH2	2:C:456:ALA:O	2.32	0.62
2:M:727:PRO:HB3	2:M:783:ARG:HD3	1.82	0.61
3:N:208:PRO:HA	3:N:390:PRO:HA	1.82	0.61
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.81	0.61
3:N:643:GLY:HA3	3:N:727:GLN:HB2	1.83	0.61
1:L:56:VAL:HG22	1:L:142:VAL:HG12	1.83	0.61
2:C:324:ASP:HB3	2:C:327:HIS:HB2	1.82	0.61
1:A:106:PRO:HG3	1:A:134:GLU:HG2	1.82	0.61
3:D:356:PRO:HG2	3:D:359:ALA:HB2	1.82	0.60
2:M:420:ARG:NH2	5:P:324:GLU:OE2	2.35	0.60
2:M:740:GLU:OE1	2:M:805:ARG:NH1	2.34	0.60
5:P:365:GLU:HB2	5:P:404:ALA:HB2	1.84	0.60
1:A:55:SER:HB3	1:A:143:ARG:HB3	1.82	0.60
3:N:65:ARG:NH1	5:P:378:GLY:O	2.35	0.60
3:N:356:PRO:HG2	3:N:359:ALA:HB2	1.83	0.59
2:C:715:THR:OG1	2:C:718:GLY:O	2.19	0.59
3:D:260:GLU:OE1	3:D:273:ARG:NH1	2.35	0.59
2:C:586:ARG:NH2	2:C:590:ASP:OD1	2.36	0.59
3:D:1045:MET:HE2	3:D:1073:SER:HA	1.83	0.59
5:F:193:ARG:HB2	6:H:6:DT:H1'	1.84	0.59
3:N:366:LYS:HD3	3:N:369:ALA:HB2	1.84	0.59
2:C:637:LEU:HG	2:C:659:PRO:HG3	1.83	0.59
4:O:39:VAL:O	4:O:72:ARG:NH1	2.31	0.59
2:C:462:ASP:OD2	2:C:468:ARG:NH1	2.34	0.59
2:C:266:ARG:NH1	6:H:11:DG:O6	2.35	0.59
3:D:1168:MET:HE3	3:D:1168:MET:HA	1.84	0.59
3:N:128:TYR:OH	3:N:579:ASP:OD2	2.20	0.59
3:N:569:ASN:ND2	5:P:214:GLN:OE1	2.35	0.59
2:C:64:LEU:HD12	2:C:103:LYS:HB2	1.85	0.59
3:D:685:ASP:HA	3:D:688:TRP:HD1	1.66	0.59
3:D:1461:GLY:O	3:D:1465:ASN:ND2	2.36	0.58
2:C:758:ARG:HH21	2:C:788:THR:HB	1.67	0.58
3:D:954:ALA:O	3:D:1062:ARG:NH2	2.35	0.58
1:A:58:ILE:HG12	1:A:140:MET:HG2	1.85	0.58
3:D:1236:LEU:HA	3:D:1359:GLN:HG3	1.85	0.58
2:C:202:TYR:OH	2:C:300:ASP:OD1	2.20	0.58
2:C:232:GLU:HG3	2:C:250:ARG:HE	1.69	0.58
1:A:218:LEU:HD23	1:B:222:LEU:HD21	1.85	0.58
3:D:273:ARG:HB3	3:D:278:PRO:HA	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:807:ARG:NH1	13:M:1205:HOH:O	2.37	0.58
3:N:704:ARG:NH2	10:N:1604:C5P:O2'	2.36	0.58
2:C:172:ILE:HG12	2:C:186:VAL:HG22	1.86	0.58
2:C:710:ILE:HD12	2:C:790:LEU:HB2	1.85	0.58
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.85	0.58
3:D:787:LEU:HD21	3:D:947:ILE:HG21	1.85	0.57
2:M:172:ILE:HG12	2:M:186:VAL:HG22	1.85	0.57
3:N:1047:LYS:HD3	3:N:1051:GLU:HB3	1.87	0.57
2:M:17:PRO:HB2	2:M:20:GLU:HB3	1.86	0.57
3:N:787:LEU:HD21	3:N:947:ILE:HG21	1.87	0.57
3:D:1040:GLY:O	3:D:1060:SER:HB3	2.05	0.57
2:M:92:ALA:HB2	2:M:120:LEU:HD11	1.86	0.57
5:F:131:VAL:HG13	5:F:178:ARG:HD3	1.86	0.57
3:D:996:TRP:CD2	3:D:1056:PRO:HG3	2.40	0.57
2:M:324:ASP:O	2:M:330:ASN:ND2	2.29	0.57
2:C:283:ILE:HD13	2:C:305:PRO:HG2	1.86	0.56
2:M:715:THR:OG1	2:M:718:GLY:O	2.23	0.56
2:C:12:VAL:HG13	2:C:13:ILE:HG23	1.87	0.56
3:N:474:GLU:HG3	3:N:496:LEU:HD11	1.88	0.56
1:L:11:PHE:HE1	1:L:23:PHE:HB3	1.69	0.56
1:B:92:PRO:O	1:B:146:ARG:NH2	2.39	0.56
5:P:210:LEU:HD23	5:P:213:ILE:HD12	1.87	0.56
1:K:222:LEU:HD21	1:L:218:LEU:HD23	1.89	0.55
5:P:131:VAL:HG13	5:P:178:ARG:HD3	1.88	0.55
2:M:768:THR:OG1	2:M:771:GLU:OE1	2.25	0.55
3:D:474:GLU:HG3	3:D:496:LEU:HD11	1.88	0.55
5:P:188:ILE:HD13	5:P:221:ILE:HG12	1.88	0.55
2:C:428:ARG:NH2	2:C:447:ALA:O	2.32	0.55
5:F:360:LYS:HG3	5:F:411:HIS:HB2	1.88	0.55
3:N:266:GLU:HG3	3:N:314:PRO:HB3	1.88	0.55
3:N:1296:SER:HB3	3:N:1299:PHE:HB2	1.88	0.55
5:P:120:THR:HG22	5:P:122:LEU:HD13	1.90	0.54
2:C:24:GLU:HG3	2:C:27:ARG:HH22	1.72	0.54
2:C:399:ASN:O	2:C:402:SER:OG	2.22	0.54
2:M:207:LEU:HD13	2:M:221:LEU:HD21	1.89	0.54
1:A:24:VAL:HG22	1:A:196:THR:HG23	1.88	0.54
5:F:284:ARG:NH2	5:F:290:GLU:OE2	2.38	0.54
2:C:207:LEU:HD13	2:C:221:LEU:HD21	1.89	0.54
2:M:168:ARG:HE	2:M:168:ARG:HA	1.73	0.54
3:D:904:VAL:HG22	3:D:905:PRO:HD2	1.89	0.54
3:D:1495:ILE:HG21	4:E:80:VAL:HG12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:703:ASN:HB2	3:N:713:ILE:HG12	1.89	0.54
3:D:266:GLU:HG3	3:D:314:PRO:HB3	1.90	0.54
3:D:1042:ARG:HB3	3:D:1057:VAL:HB	1.90	0.54
1:L:80:LEU:HD21	3:N:842:VAL:HG12	1.90	0.54
3:N:284:LEU:HD22	3:N:288:MET:HE2	1.90	0.54
3:D:734:GLU:OE2	3:D:780:LYS:NZ	2.40	0.54
3:N:1152:GLU:HG2	3:N:1162:GLU:H	1.72	0.54
3:N:172:PRO:HG2	3:N:175:VAL:HB	1.90	0.53
1:B:108:GLU:HG2	1:B:131:THR:HG22	1.89	0.53
2:C:714:ASP:OD2	2:C:808:ARG:NH1	2.41	0.53
3:D:563:PRO:HD2	3:D:566:ILE:HD12	1.89	0.53
3:D:1020:LEU:HB3	3:D:1035:ILE:HD12	1.89	0.53
3:N:685:ASP:HA	3:N:688:TRP:HD1	1.72	0.53
2:C:39:ARG:NH1	2:C:71:TYR:O	2.29	0.53
3:D:231:VAL:O	3:D:236:TYR:OH	2.26	0.53
2:M:361:MET:HE1	5:P:201:LYS:HD2	1.89	0.53
2:C:55:GLU:O	2:C:356:ARG:NH2	2.41	0.53
3:D:242:LEU:HB3	3:D:311:LEU:HD12	1.89	0.53
3:D:707:THR:HG23	3:D:712:GLY:HA3	1.91	0.53
3:D:1044:LEU:HD23	3:D:1056:PRO:HB3	1.90	0.53
3:D:1047:LYS:HD3	3:D:1051:GLU:HG3	1.90	0.53
5:F:120:THR:HG22	5:F:122:LEU:HD13	1.91	0.53
2:M:283:ILE:HD13	2:M:305:PRO:HG2	1.91	0.53
2:M:758:ARG:HH21	2:M:788:THR:HB	1.72	0.53
3:N:353:VAL:HG11	3:N:387:LEU:HD11	1.90	0.53
1:B:56:VAL:HG22	1:B:142:VAL:HG12	1.90	0.53
2:C:754:ILE:HG12	2:C:791:ARG:HG2	1.90	0.53
3:N:238:PRO:HD3	3:N:318:ARG:HG2	1.89	0.53
2:C:900:ARG:NH1	13:C:1206:HOH:O	2.42	0.53
3:D:809:PRO:HB3	3:D:839:LEU:HD13	1.90	0.53
3:N:644:LEU:HD12	3:N:645:PRO:HD2	1.89	0.53
3:D:520:LEU:O	3:D:525:ARG:NE	2.39	0.53
2:M:1110:ASP:OD2	2:M:1114:GLY:N	2.33	0.53
2:C:370:ALA:O	5:F:280:GLN:NE2	2.38	0.53
2:M:462:ASP:HB3	2:M:468:ARG:HD2	1.91	0.53
1:K:59:GLU:OE1	1:K:139:ASN:ND2	2.37	0.53
3:N:1044:LEU:HD23	3:N:1056:PRO:HB3	1.90	0.53
2:M:937:ASP:OD1	2:M:939:ARG:HD3	2.09	0.52
3:N:132:TYR:OH	3:N:568:ARG:NH1	2.43	0.52
2:C:223:ASP:OD1	2:C:225:SER:OG	2.25	0.52
2:C:1019:GLN:HG2	2:C:1058:ASP:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:188:ILE:HG12	5:F:224:VAL:HG21	1.90	0.52
2:M:413:LEU:HD21	2:M:451:LEU:HD13	1.90	0.52
3:N:1003:VAL:HG21	3:N:1041:LEU:HG	1.91	0.52
2:C:1038:TRP:CE2	3:D:1099:VAL:HG11	2.44	0.52
2:M:936:VAL:HG11	2:M:959:PRO:HB2	1.91	0.52
3:N:351:MET:HG2	3:N:370:ALA:CB	2.39	0.52
2:C:254:VAL:O	2:C:258:TYR:HB3	2.10	0.52
2:M:13:ILE:HD13	2:M:483:VAL:HG11	1.91	0.52
2:C:950:LEU:HB3	2:C:952:LEU:HD13	1.90	0.52
3:D:114:THR:HG23	3:D:495:ARG:HG2	1.91	0.52
2:M:223:ASP:OD1	2:M:225:SER:OG	2.26	0.52
3:N:356:PRO:HB3	3:N:441:ARG:HA	1.92	0.52
2:C:936:VAL:HG11	2:C:959:PRO:HB2	1.92	0.52
2:C:413:LEU:HD21	2:C:451:LEU:HD13	1.92	0.51
2:C:504:GLU:HG2	2:C:509:ALA:HB2	1.91	0.51
5:F:361:LEU:HD13	5:F:407:LYS:HD2	1.92	0.51
1:L:108:GLU:HG2	1:L:131:THR:HG22	1.92	0.51
2:M:571:LEU:HB2	2:M:574:ALA:HB2	1.92	0.51
3:N:1374:GLN:NE2	13:N:2104:HOH:O	2.42	0.51
2:C:657:ASP:OD2	2:C:663:ASN:N	2.44	0.51
3:N:575:GLN:NE2	3:N:579:ASP:OD1	2.43	0.51
3:N:956:ILE:HD11	3:N:1062:ARG:HG2	1.90	0.51
2:M:160:ALA:HB3	2:M:174:LEU:HB2	1.92	0.51
5:F:370:LYS:HG2	5:F:375:LEU:HD22	1.93	0.51
3:N:1101:VAL:HG13	3:N:1102:THR:HG23	1.91	0.51
3:D:256:GLU:HG2	3:D:299:GLU:HA	1.92	0.51
3:D:647:ARG:HH21	3:D:724:GLN:HG2	1.76	0.51
3:D:1350:GLU:OE2	3:D:1357:ARG:NH1	2.40	0.51
2:M:41:ASN:O	2:M:46:ALA:HB2	2.11	0.51
3:N:633:VAL:HB	3:N:740:PHE:CE2	2.45	0.51
1:B:176:ARG:NH2	3:D:888:GLU:OE1	2.44	0.51
2:C:460:ARG:HD3	2:C:485:TYR:CE2	2.46	0.51
2:C:971:LYS:HB3	2:C:986:PRO:HB2	1.93	0.51
3:D:1101:VAL:HG13	3:D:1102:THR:HG23	1.93	0.51
7:G:14:DA:H2'	7:G:15:DG:C8	2.45	0.51
3:N:895:VAL:HG11	3:N:922:LEU:HD21	1.93	0.51
3:N:1236:LEU:HA	3:N:1359:GLN:HG3	1.93	0.51
2:C:800:VAL:HG22	2:C:827:VAL:HG22	1.92	0.51
3:D:956:ILE:HD11	3:D:1062:ARG:HG2	1.93	0.51
2:M:1008:ARG:NH2	13:M:1203:HOH:O	2.33	0.51
3:N:455:ARG:HB2	3:N:460:ALA:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:168:ARG:O	2:C:267:TYR:HA	2.11	0.50
2:M:847:GLY:HA2	3:N:741:ASP:HA	1.93	0.50
2:M:1038:TRP:CE2	3:N:1099:VAL:HG11	2.46	0.50
5:F:152:ASP:N	5:F:152:ASP:OD1	2.43	0.50
2:M:711:GLU:HG2	2:M:822:VAL:HG22	1.92	0.50
2:M:787:ASP:OD2	2:M:791:ARG:NH2	2.40	0.50
1:B:80:LEU:HD21	3:D:842:VAL:HG12	1.93	0.50
3:D:1068:LEU:O	3:D:1072:ILE:HG12	2.12	0.50
5:P:188:ILE:HG12	5:P:224:VAL:HG21	1.94	0.50
3:D:658:LEU:HA	3:D:661:MET:HE3	1.93	0.50
3:N:809:PRO:HB3	3:N:839:LEU:HD13	1.93	0.50
5:F:135:ILE:HG13	5:F:181:GLU:HB2	1.93	0.50
3:N:840:LYS:HE3	3:N:841:TYR:CZ	2.47	0.50
3:D:633:VAL:C	3:D:635:PRO:HD3	2.37	0.50
3:N:314:PRO:HB2	3:N:317:VAL:HG12	1.94	0.50
2:C:712:ALA:HB3	2:C:821:GLU:HG3	1.94	0.50
2:C:808:ARG:NH2	5:F:305:GLU:OE2	2.45	0.49
3:D:407:VAL:HG22	3:D:409:VAL:H	1.77	0.49
2:M:670:GLN:HG2	2:M:699:PHE:CD2	2.47	0.49
3:N:899:LEU:HD22	3:N:917:GLN:HB3	1.93	0.49
2:C:122:THR:HG22	2:C:123:GLU:H	1.76	0.49
1:K:196:THR:HG21	2:M:934:PHE:HE1	1.77	0.49
3:N:637:LEU:HD13	3:N:642:CYS:HA	1.94	0.49
2:C:111:ASP:OD1	2:C:112:GLU:N	2.45	0.49
2:C:513:VAL:HG13	2:C:524:VAL:HG23	1.94	0.49
3:D:192:ALA:HB3	3:D:195:VAL:HB	1.95	0.49
3:N:661:MET:HE3	3:N:673:ALA:HB1	1.95	0.49
3:N:890:VAL:HB	3:N:922:LEU:HD13	1.93	0.49
2:M:168:ARG:O	2:M:267:TYR:HA	2.12	0.49
2:M:1067:TYR:OH	3:N:674:ARG:NH1	2.42	0.49
2:C:285:LEU:HD21	2:C:302:VAL:HG22	1.95	0.49
3:N:500:ARG:NH1	3:N:1388:ARG:O	2.44	0.49
3:D:241:ILE:HG12	3:D:310:LEU:HD21	1.95	0.49
2:M:843:HIS:NE2	2:M:887:GLU:OE2	2.41	0.49
1:A:36:LEU:HD11	1:B:221:HIS:HB3	1.95	0.49
1:A:65:PHE:HE1	2:C:703:ILE:HD12	1.78	0.49
1:B:138:LEU:HD11	1:B:140:MET:HE3	1.95	0.49
2:C:331:ARG:NH1	13:C:1205:HOH:O	2.37	0.49
3:D:664:LYS:HB2	3:D:666:ILE:HD12	1.94	0.49
3:N:975:GLU:O	3:N:979:GLU:HG2	2.12	0.49
1:A:6:LEU:HD11	1:A:27:PRO:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:410:TYR:O	5:F:413:SER:OG	2.29	0.48
2:M:1009:SER:HB3	3:N:651:GLU:O	2.12	0.48
2:C:299:LYS:HE3	2:C:300:ASP:H	1.77	0.48
2:M:390:GLN:HB3	2:M:415:PRO:HD3	1.96	0.48
2:C:886:LEU:HD21	3:D:951:ILE:HG12	1.95	0.48
3:D:261:LEU:HD13	3:D:270:LEU:HD12	1.95	0.48
2:M:229:MET:HB2	2:M:233:GLU:HB2	1.96	0.48
2:M:674:VAL:HG12	2:M:869:VAL:HB	1.96	0.48
2:C:164:PRO:HA	2:C:269:LEU:HD23	1.95	0.48
2:C:390:GLN:HG2	2:C:414:GLY:HA2	1.94	0.48
5:F:153:PRO:HA	5:F:156:VAL:HG22	1.96	0.48
3:N:106:LYS:O	3:N:586:ARG:NH1	2.46	0.48
3:N:192:ALA:HB3	3:N:195:VAL:HB	1.96	0.48
3:N:1068:LEU:O	3:N:1072:ILE:HG12	2.13	0.48
2:C:937:ASP:OD1	2:C:939:ARG:HD3	2.14	0.48
10:N:1604:C5P:O2	7:R:15:DG:N2	2.37	0.48
2:C:32:ALA:HB2	2:C:73:LEU:HD12	1.95	0.48
2:M:911:GLU:O	2:M:915:LYS:HG2	2.14	0.48
1:A:179:PHE:HB3	1:A:197:LEU:HD23	1.96	0.48
1:K:25:LEU:HD23	1:K:28:LEU:HD11	1.96	0.48
1:L:92:PRO:O	1:L:146:ARG:NH2	2.46	0.48
3:N:162:ARG:O	3:N:449:SER:HB2	2.14	0.48
2:C:41:ASN:O	2:C:46:ALA:HB2	2.14	0.48
3:D:50:PHE:O	3:D:89:ARG:HD2	2.14	0.48
5:P:270:LYS:HG2	5:P:295:MET:HE1	1.96	0.48
1:B:38:ASN:ND2	2:C:978:ARG:O	2.46	0.48
3:D:272:LEU:HB2	3:D:280:ALA:HB3	1.96	0.48
2:C:87:ASP:HA	2:C:131:GLY:HA3	1.96	0.47
2:M:281:LEU:HD13	2:M:305:PRO:HB2	1.96	0.47
3:N:307:ALA:HB1	3:N:311:LEU:HD11	1.96	0.47
5:F:370:LYS:HB3	5:F:375:LEU:HB2	1.96	0.47
2:C:324:ASP:O	2:C:330:ASN:ND2	2.45	0.47
5:F:383:LEU:H	5:F:383:LEU:HD22	1.79	0.47
2:M:711:GLU:O	2:M:758:ARG:NH1	2.46	0.47
3:N:1353:GLN:NE2	3:N:1365:ASP:OD1	2.46	0.47
5:P:93:LEU:HD21	5:P:193:ARG:HD2	1.95	0.47
1:K:179:PHE:HB3	1:K:197:LEU:HD23	1.96	0.47
2:M:708:TYR:OH	2:M:796:GLU:OE1	2.31	0.47
2:C:599:GLU:HG3	2:C:600:ASP:H	1.79	0.47
1:L:83:LYS:HE2	1:L:168:ASP:HB2	1.95	0.47
1:L:8:ALA:HB1	1:L:9:PRO:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:GLU:HG2	1:A:76:VAL:HG22	1.96	0.47
2:C:261:ILE:HD11	2:C:303:PHE:CZ	2.48	0.47
2:C:773:LEU:HD23	5:F:354:LEU:HD13	1.96	0.47
1:K:216:GLU:OE2	1:K:219:ARG:NH2	2.48	0.47
2:M:1104:GLU:HG2	3:N:6:ARG:HG3	1.97	0.47
3:N:368:VAL:HB	3:N:377:VAL:HB	1.96	0.47
3:N:954:ALA:O	3:N:1062:ARG:NH2	2.47	0.47
3:N:1105:ILE:HG23	3:N:1199:GLY:HA2	1.96	0.47
3:N:1168:MET:HA	3:N:1168:MET:HE3	1.95	0.47
10:N:1604:C5P:C2	7:R:15:DG:H22	2.26	0.47
5:P:144:ILE:HB	5:P:147:LEU:HD13	1.96	0.47
5:P:212:LEU:HD22	5:P:247:ILE:HG23	1.95	0.47
2:C:470:PRO:HG3	2:C:485:TYR:CE2	2.50	0.47
3:D:97:THR:HG21	3:D:571:LYS:HG2	1.96	0.47
3:D:1147:ARG:NH2	3:D:1369:GLU:OE1	2.43	0.47
2:M:740:GLU:HB3	2:M:805:ARG:HH12	1.79	0.47
3:N:166:GLN:HB3	3:N:396:VAL:HG13	1.97	0.47
3:D:1285:GLU:HG3	3:D:1290:LEU:HG	1.97	0.47
1:K:218:LEU:HD23	1:L:222:LEU:HD21	1.96	0.47
1:A:210:ALA:HA	1:A:213:GLN:HE21	1.80	0.46
10:D:2005:C5P:C2	7:G:15:DG:H22	2.28	0.46
3:D:417:PRO:HG3	3:D:431:VAL:HA	1.97	0.46
1:L:128:HIS:CE1	1:L:131:THR:HG23	2.51	0.46
3:N:797:LYS:HE3	3:N:826:PRO:HG3	1.98	0.46
3:D:162:ARG:O	3:D:449:SER:HB2	2.15	0.46
2:M:617:ASP:HB2	2:M:619:ARG:HG2	1.97	0.46
3:D:284:LEU:HD22	3:D:288:MET:HE2	1.96	0.46
3:D:704:ARG:HB2	3:D:745:MET:HE2	1.97	0.46
5:F:386:VAL:HG13	5:F:397:ILE:HG21	1.98	0.46
1:B:78:ILE:HG21	1:B:140:MET:HE1	1.97	0.46
3:D:750:PRO:HG2	3:D:756:GLN:NE2	2.30	0.46
1:A:57:TYR:HE1	1:A:163:ASN:HB2	1.81	0.46
2:C:390:GLN:HB3	2:C:415:PRO:HD3	1.97	0.46
5:F:414:ARG:HG2	5:F:415:THR:HG23	1.98	0.46
2:C:267:TYR:CE1	2:C:290:LEU:HG	2.50	0.46
5:F:412:GLU:O	5:F:416:ARG:N	2.43	0.46
1:K:24:VAL:HG22	1:K:196:THR:HG23	1.98	0.46
1:K:209:GLU:O	1:K:213:GLN:HG2	2.16	0.46
1:L:55:SER:HB3	1:L:143:ARG:HB3	1.96	0.46
3:N:822:ALA:HB3	3:N:825:ALA:HB2	1.98	0.46
2:C:105:THR:HG22	2:C:107:LEU:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:26:GLU:HB3	1:K:194:LYS:HG3	1.97	0.46
1:L:78:ILE:HG21	1:L:140:MET:HE1	1.96	0.46
2:M:1095:LEU:HD23	3:N:582:LEU:HD22	1.98	0.46
3:N:606:ILE:O	3:N:613:ARG:N	2.49	0.46
3:D:1379:VAL:HG21	3:D:1400:VAL:HG11	1.98	0.46
5:F:392:VAL:HG12	5:F:393:THR:H	1.81	0.46
2:M:419:THR:HG23	2:M:422:ARG:HG3	1.98	0.45
3:N:707:THR:HG23	3:N:712:GLY:HA3	1.99	0.45
3:N:1102:THR:HG21	3:N:1371:VAL:HG22	1.98	0.45
2:C:470:PRO:HB2	2:C:534:VAL:HG21	1.98	0.45
1:K:70:GLY:N	2:M:607:ASP:OD1	2.50	0.45
3:N:850:LEU:HD12	3:N:884:ARG:NH2	2.31	0.45
5:P:373:LYS:HA	5:P:373:LYS:HD3	1.85	0.45
3:D:487:ALA:O	3:D:491:LYS:HG2	2.16	0.45
5:F:93:LEU:HD21	5:F:193:ARG:HD2	1.97	0.45
3:D:356:PRO:HB3	3:D:441:ARG:HA	1.99	0.45
3:N:224:ARG:NE	3:N:254:GLU:OE2	2.40	0.45
1:B:77:GLU:OE1	3:D:867:ARG:NH2	2.44	0.45
3:D:22:SER:HB2	3:D:92:HIS:HB3	1.99	0.45
3:D:1364:HIS:ND1	3:D:1366:LYS:HG2	2.32	0.45
1:A:216:GLU:OE2	1:A:219:ARG:NH2	2.50	0.45
3:D:101:HIS:HB3	3:D:104:PHE:HD2	1.82	0.45
1:K:133:GLU:HG2	1:K:134:GLU:H	1.81	0.45
3:N:1216:SER:N	13:N:2117:HOH:O	2.50	0.45
5:P:80:PRO:HB2	5:P:210:LEU:HD11	1.99	0.45
3:D:248:PRO:HG3	3:D:308:LYS:HE3	1.98	0.45
3:D:314:PRO:HB2	3:D:317:VAL:HG12	1.98	0.45
1:L:90:LEU:HD13	1:L:90:LEU:HA	1.75	0.45
2:M:324:ASP:HB3	2:M:327:HIS:HB2	1.99	0.45
2:M:390:GLN:HG2	2:M:414:GLY:HA2	1.98	0.45
2:M:425:PHE:CE1	3:N:1086:LEU:HD12	2.52	0.45
2:M:504:GLU:HG2	2:M:509:ALA:HB2	1.99	0.45
5:P:187:LEU:HD23	5:P:224:VAL:HG13	1.97	0.45
3:D:890:VAL:HG23	3:D:892:ASP:H	1.81	0.45
3:N:633:VAL:O	3:N:635:PRO:HD3	2.17	0.45
5:P:193:ARG:HB2	6:S:6:DT:H1'	1.98	0.45
3:D:285:PRO:HD2	3:D:288:MET:SD	2.57	0.45
5:F:205:ARG:HG3	5:F:251:ILE:HD13	1.99	0.45
2:M:708:TYR:HB3	2:M:790:LEU:HD21	1.99	0.45
2:M:950:LEU:HB3	2:M:952:LEU:HD13	1.99	0.44
3:N:685:ASP:HA	3:N:688:TRP:CD1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:153:PRO:HA	5:P:156:VAL:HG22	1.98	0.44
2:C:469:THR:HA	2:C:470:PRO:HD3	1.88	0.44
2:C:1009:SER:HB3	3:D:651:GLU:O	2.17	0.44
3:D:67:ARG:CZ	5:F:379:ARG:HD2	2.47	0.44
1:K:53:VAL:HG22	1:K:144:VAL:HG22	1.99	0.44
2:M:678:PRO:HA	2:M:683:ASN:HD21	1.82	0.44
3:N:629:SER:HB3	3:N:726:ILE:HG13	1.99	0.44
5:P:193:ARG:HB3	6:S:7:DG:H5''	1.98	0.44
3:D:834:THR:OG1	3:D:835:SER:N	2.49	0.44
3:D:1500:LYS:HE2	3:D:1500:LYS:HB3	1.79	0.44
6:H:10:DA:H2''	6:H:11:DG:C8	2.53	0.44
3:N:42:ASP:OD1	3:N:48:ARG:NH1	2.50	0.44
3:N:407:VAL:HG22	3:N:409:VAL:H	1.81	0.44
2:C:353:ARG:NH2	5:F:203:THR:OG1	2.50	0.44
3:D:644:LEU:HD12	3:D:645:PRO:HD2	1.98	0.44
1:L:77:GLU:OE1	3:N:867:ARG:NH2	2.41	0.44
2:M:535:SER:O	2:M:538:GLN:HG2	2.17	0.44
5:P:234:LYS:HG3	6:S:4:DA:H3'	1.99	0.44
3:D:397:LYS:HE2	3:D:397:LYS:HB3	1.86	0.44
2:M:40:GLU:O	2:M:45:GLN:HG2	2.17	0.44
2:M:177:GLU:HG3	2:M:178:PRO:HD2	2.00	0.44
2:M:607:ASP:HB2	2:M:610:ARG:HH11	1.82	0.44
3:D:14:SER:HB3	3:D:511:TRP:CE2	2.52	0.44
3:D:864:VAL:HG22	3:D:865:THR:H	1.83	0.44
2:M:224:GLU:CD	2:M:224:GLU:H	2.26	0.44
1:A:53:VAL:HG22	1:A:144:VAL:HG22	2.00	0.44
2:C:22:GLN:HG3	2:C:407:LYS:HB3	2.00	0.44
3:D:171:LEU:HD12	3:D:390:PRO:HG2	2.00	0.44
3:D:371:ILE:HG23	5:F:230:LYS:HD2	1.99	0.44
1:L:111:ALA:HB3	1:L:125:PRO:HA	1.98	0.44
2:M:610:ARG:HG2	2:M:611:ILE:N	2.33	0.44
2:C:684:PHE:HB3	3:D:633:VAL:HG21	2.00	0.43
2:C:1110:ASP:OD2	2:C:1114:GLY:N	2.32	0.43
3:D:520:LEU:HD12	3:D:521:PRO:HD2	2.00	0.43
3:D:555:LYS:HA	5:F:142:ARG:HH12	1.83	0.43
1:K:150:TYR:CD1	2:M:696:LYS:HG2	2.53	0.43
2:M:605:LYS:HB2	2:M:612:VAL:HB	1.99	0.43
3:N:1377:LYS:HE3	3:N:1378:TYR:CZ	2.53	0.43
3:D:1283:ILE:H	3:D:1283:ILE:HG13	1.70	0.43
6:H:16:DC:H2''	6:H:17:DA:H5'	1.99	0.43
1:K:91:ASN:HA	1:K:92:PRO:HD3	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:101:HIS:HB3	3:N:104:PHE:HD2	1.82	0.43
5:P:163:LEU:HD13	5:P:174:LEU:HD13	2.00	0.43
1:B:64:GLU:HA	1:B:165:ILE:HD13	2.01	0.43
2:C:1003:ASP:O	2:C:1024:LYS:NZ	2.44	0.43
3:D:39:PRO:HG2	3:D:47:GLU:HG3	2.00	0.43
2:C:766:GLU:HG2	3:D:65:ARG:HE	1.83	0.43
2:M:226:VAL:HA	2:M:229:MET:HE2	2.00	0.43
3:N:569:ASN:O	3:N:573:MET:HG3	2.19	0.43
3:N:619:LEU:HD11	3:N:1439:SER:HB2	2.00	0.43
5:P:279:GLN:HB3	5:P:286:PRO:HD3	1.99	0.43
2:C:420:ARG:C	2:C:422:ARG:H	2.27	0.43
1:L:71:VAL:HG22	1:L:132:LEU:HG	2.00	0.43
2:M:172:ILE:HD13	2:M:184:MET:HE3	2.00	0.43
2:M:675:ALA:HB2	2:M:867:VAL:HG11	1.99	0.43
3:N:864:VAL:HG22	3:N:865:THR:H	1.82	0.43
1:A:102:LYS:HE3	1:A:102:LYS:HB2	1.89	0.43
1:A:112:ARG:HG3	1:A:125:PRO:HB2	2.01	0.43
3:D:200:ASP:O	3:D:397:LYS:HG2	2.17	0.43
3:D:610:LYS:HA	3:D:615:ARG:HD3	2.00	0.43
4:O:3:GLU:HB3	4:O:65:MET:HE1	2.01	0.43
2:C:389:SER:OG	2:C:390:GLN:N	2.52	0.43
3:D:923:GLY:O	3:D:927:THR:OG1	2.31	0.43
2:C:1051:GLU:HG3	2:C:1055:LEU:HD12	2.01	0.43
3:D:142:LEU:HB2	3:D:161:LEU:HD11	2.00	0.43
3:D:1381:VAL:HG21	3:D:1389:LEU:HD23	1.99	0.43
4:E:40:LEU:HG	4:E:67:GLU:HG2	2.01	0.43
5:F:144:ILE:HB	5:F:147:LEU:HD13	2.00	0.43
3:N:114:THR:HG23	3:N:495:ARG:HG2	2.01	0.43
3:N:472:ALA:O	3:N:476:GLU:HG2	2.18	0.43
2:C:12:VAL:HG11	2:C:472:ARG:HD3	2.01	0.43
2:C:584:GLU:OE2	2:C:584:GLU:N	2.52	0.43
4:E:83:ASP:O	4:E:87:LYS:HG2	2.19	0.43
4:E:13:VAL:HG21	4:E:19:LEU:HB2	2.00	0.43
2:M:210:GLU:HG2	2:M:304:LEU:HD21	2.00	0.43
3:N:483:HIS:CG	3:N:484:PRO:HD2	2.53	0.43
5:P:323:ASP:OD1	5:P:323:ASP:N	2.31	0.43
1:A:133:GLU:HG2	1:A:134:GLU:H	1.84	0.42
1:A:209:GLU:O	1:A:213:GLN:HG2	2.19	0.42
1:B:124:ASN:OD1	1:B:124:ASN:N	2.52	0.42
1:B:150:TYR:CE2	1:B:170:VAL:HG22	2.54	0.42
2:C:471:TYR:CD2	2:C:486:MET:HE3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:187:LYS:N	3:D:200:ASP:OD2	2.43	0.42
3:D:236:TYR:HB3	3:D:313:MET:HG3	2.01	0.42
3:D:729:HIS:HA	3:D:730:PRO:HD3	1.93	0.42
3:D:741:ASP:OD1	3:D:741:ASP:N	2.48	0.42
3:D:935:LYS:HE2	3:D:935:LYS:HB3	1.88	0.42
5:F:323:ASP:OD1	5:F:323:ASP:N	2.52	0.42
1:K:87:VAL:HG21	1:K:144:VAL:HG21	2.00	0.42
2:M:848:VAL:HG22	3:N:740:PHE:O	2.19	0.42
1:A:226:SER:O	1:A:228:PRO:HD3	2.19	0.42
2:C:146:VAL:HG21	2:C:281:LEU:HD11	2.01	0.42
2:C:249:LYS:HB3	2:C:249:LYS:HE2	1.85	0.42
2:C:911:GLU:O	2:C:915:LYS:HG2	2.19	0.42
2:M:35:PRO:HA	2:M:36:PRO:HD3	1.89	0.42
3:N:137:PRO:HD3	3:N:149:LYS:HG3	2.01	0.42
3:N:715:ALA:HB3	3:N:764:LEU:HA	2.00	0.42
5:P:285:GLU:HA	5:P:286:PRO:HD3	1.81	0.42
1:B:94:LEU:O	1:B:146:ARG:NH2	2.49	0.42
2:C:247:PRO:HA	2:C:248:PRO:HD3	1.75	0.42
3:D:355:VAL:HG11	3:D:385:VAL:HG21	2.00	0.42
3:D:1124:GLN:OE1	3:D:1133:ARG:NH1	2.52	0.42
1:L:104:GLU:OE2	1:L:137:ARG:NH1	2.53	0.42
2:M:12:VAL:HG21	2:M:472:ARG:HD3	2.01	0.42
3:N:1040:GLY:O	3:N:1060:SER:HB3	2.19	0.42
3:N:1462:LEU:HD22	3:N:1472:ILE:HB	2.01	0.42
2:C:1090:LYS:HA	2:C:1090:LYS:HD3	1.86	0.42
2:C:1106:ASP:OD1	3:D:7:LYS:NZ	2.44	0.42
3:D:181:ASP:HB2	3:D:205:TYR:CD2	2.54	0.42
3:D:259:VAL:HG22	3:D:272:LEU:HD11	2.01	0.42
3:D:500:ARG:NH1	3:D:1388:ARG:O	2.41	0.42
3:D:764:LEU:O	3:D:768:ASN:ND2	2.53	0.42
2:M:879:ARG:NH1	13:M:1216:HOH:O	2.52	0.42
3:N:1344:VAL:HG11	3:N:1421:LEU:HD22	2.01	0.42
3:D:850:LEU:HD12	3:D:884:ARG:NH2	2.35	0.42
5:F:222:ARG:NH2	5:F:225:GLU:OE1	2.52	0.42
5:F:414:ARG:HG2	5:F:415:THR:N	2.34	0.42
2:M:602:GLU:HB2	2:M:648:ARG:HH21	1.84	0.42
2:M:905:ILE:C	2:M:907:ASP:H	2.27	0.42
3:N:179:VAL:O	3:N:205:TYR:OH	2.35	0.42
3:N:1000:THR:HG23	3:N:1036:ARG:HD2	2.01	0.42
6:S:10:DA:H2"	6:S:11:DG:C8	2.55	0.42
2:C:35:PRO:HA	2:C:36:PRO:HD3	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:167:GLU:OE2	3:D:198:ARG:NH1	2.53	0.42
3:D:372:ASP:HA	3:D:373:PRO:HD3	1.87	0.42
3:D:472:ALA:O	3:D:476:GLU:HG2	2.20	0.42
3:D:317:VAL:HG23	3:D:339:TRP:HB3	2.02	0.42
3:D:353:VAL:HG12	3:D:355:VAL:H	1.85	0.42
3:D:684:LYS:HE2	3:D:684:LYS:HB3	1.86	0.42
2:M:299:LYS:HB2	2:M:299:LYS:HE3	1.84	0.42
3:N:72:VAL:HA	3:N:79:GLU:HA	2.02	0.42
3:N:129:PHE:CD2	3:N:456:MET:HB3	2.54	0.42
5:P:333:ILE:HA	5:P:334:PRO:HD3	1.82	0.42
6:S:19:DG:H2'	6:S:20:DG:C8	2.55	0.42
2:C:631:SER:HB3	2:C:637:LEU:HD13	2.02	0.42
2:M:118:ILE:HD11	2:M:344:PHE:CE1	2.55	0.42
2:M:611:ILE:HD11	2:M:641:PRO:HB3	2.02	0.42
2:M:976:ASP:OD1	2:M:978:ARG:HD3	2.19	0.42
3:N:633:VAL:HB	3:N:740:PHE:CZ	2.54	0.42
3:N:1115:THR:O	3:N:1151:ARG:NH1	2.53	0.42
2:C:1100:GLN:HG3	3:D:9:ARG:HH21	1.85	0.42
1:L:11:PHE:CE1	1:L:23:PHE:HB3	2.52	0.42
1:L:51:THR:OG1	1:L:87:VAL:O	2.35	0.42
2:M:976:ASP:HB3	2:M:979:THR:OG1	2.20	0.42
3:N:200:ASP:O	3:N:397:LYS:HG2	2.20	0.42
3:N:256:GLU:OE1	3:N:274:ARG:NH1	2.53	0.42
3:N:1366:LYS:O	3:N:1370:ILE:HG12	2.19	0.42
3:N:1498:ALA:HB1	4:O:84:ARG:HH21	1.84	0.42
1:A:180:GLN:NE2	2:C:935:GLY:O	2.53	0.42
1:B:90:LEU:HD13	1:B:90:LEU:HA	1.79	0.42
2:C:739:GLU:CD	2:C:739:GLU:H	2.28	0.42
3:D:890:VAL:HB	3:D:922:LEU:HD13	2.02	0.42
3:D:1189:ARG:HB3	3:D:1204:CYS:HA	2.02	0.42
1:K:198:ARG:HD3	2:M:934:PHE:CZ	2.55	0.42
2:M:436:GLY:HA2	2:M:538:GLN:O	2.20	0.42
3:N:236:TYR:CD2	3:N:322:VAL:HG21	2.55	0.42
3:N:750:PRO:HG2	3:N:756:GLN:NE2	2.35	0.42
3:N:1208:ASP:HB2	3:N:1215:VAL:HA	2.02	0.42
3:N:1267:ARG:HA	3:N:1268:PRO:HD3	1.92	0.42
1:A:51:THR:OG1	1:A:87:VAL:O	2.29	0.41
2:C:285:LEU:HB3	2:C:287:GLY:O	2.20	0.41
2:C:469:THR:HG23	2:C:471:TYR:CE2	2.55	0.41
2:C:1009:SER:O	3:D:624:ASP:HB3	2.19	0.41
2:C:1043:TYR:CD2	3:D:763:MET:HG2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:238:PRO:HD3	3:D:318:ARG:HG3	2.01	0.41
3:D:245:LEU:HA	3:D:246:PRO:HD3	1.89	0.41
3:D:1487:VAL:HG22	3:D:1491:THR:HB	2.02	0.41
1:K:79:ILE:O	1:K:83:LYS:HG3	2.20	0.41
3:N:657:LEU:HG	3:N:661:MET:HE2	2.01	0.41
3:N:801:GLY:O	3:N:804:LEU:HG	2.20	0.41
3:N:809:PRO:HG3	3:N:829:VAL:HG11	2.02	0.41
5:P:338:LEU:HA	5:P:339:PRO:HD3	1.87	0.41
5:P:367:MET:HB3	5:P:390:PHE:HZ	1.85	0.41
2:C:567:GLN:O	2:C:998:TYR:N	2.53	0.41
3:D:43:GLY:H	3:D:46:ASP:HB2	1.85	0.41
3:D:90:MET:SD	3:D:521:PRO:HD3	2.61	0.41
2:M:36:PRO:HB3	2:M:70:GLU:HB2	2.02	0.41
2:C:573:ARG:NH1	2:C:697:ARG:O	2.42	0.41
2:C:670:GLN:HE22	2:C:699:PHE:HA	1.84	0.41
5:F:276:ARG:O	5:F:279:GLN:HG3	2.20	0.41
2:M:704:HIS:CE1	2:M:1000:MET:HE1	2.55	0.41
3:N:12:LEU:HD21	3:N:104:PHE:CZ	2.54	0.41
3:N:487:ALA:O	3:N:491:LYS:HG2	2.21	0.41
1:B:104:GLU:OE2	1:B:137:ARG:NH1	2.53	0.41
2:C:334:ARG:NH2	2:C:342:ASP:OD2	2.54	0.41
2:C:838:LYS:HE2	2:C:997:LEU:HD12	2.00	0.41
2:C:1090:LYS:HE2	2:C:1112:PHE:CZ	2.55	0.41
3:D:241:ILE:HD13	3:D:310:LEU:HD11	2.01	0.41
5:P:400:ILE:HA	5:P:403:LYS:HG2	2.02	0.41
2:C:168:ARG:HE	2:C:168:ARG:HA	1.85	0.41
2:C:954:THR:HA	2:C:955:PRO:HD3	1.88	0.41
3:D:65:ARG:HD3	3:D:65:ARG:HA	1.83	0.41
2:M:470:PRO:HB2	2:M:534:VAL:HG21	2.02	0.41
3:N:353:VAL:HG12	3:N:355:VAL:H	1.86	0.41
3:N:1381:VAL:HG21	3:N:1389:LEU:HD23	2.03	0.41
2:C:218:VAL:HG22	2:C:222:MET:HE2	2.03	0.41
2:C:642:ARG:HA	2:C:642:ARG:HD2	1.84	0.41
3:D:428:LYS:HE2	3:D:428:LYS:HB3	1.92	0.41
2:M:545:ASN:HB3	2:M:583:LEU:HD22	2.02	0.41
3:N:452:ILE:H	3:N:452:ILE:HG13	1.53	0.41
1:A:196:THR:HG21	2:C:934:PHE:HE1	1.84	0.41
2:C:24:GLU:HG3	2:C:27:ARG:NH2	2.35	0.41
2:C:276:LYS:HE3	2:C:276:LYS:HB3	1.92	0.41
3:D:1208:ASP:HB2	3:D:1215:VAL:HA	2.01	0.41
4:O:37:ASN:OD1	4:O:37:ASN:N	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:461:VAL:HG22	2:C:467:ILE:HG12	2.03	0.41
2:C:881:ASN:OD1	2:C:881:ASN:N	2.53	0.41
3:D:1198:TYR:OH	3:D:1432:LYS:NZ	2.47	0.41
4:E:57:ASP:HA	4:E:58:PRO:HD3	1.90	0.41
5:F:187:LEU:HD23	5:F:224:VAL:HG13	2.03	0.41
2:M:205:GLU:O	2:M:209:ARG:HG2	2.21	0.41
3:N:761:ILE:HD12	4:O:20:THR:HA	2.03	0.41
1:B:71:VAL:HG22	1:B:132:LEU:HG	2.01	0.41
1:B:153:ALA:HA	1:B:156:HIS:NE2	2.36	0.41
2:C:778:PHE:CD2	5:F:422:LEU:HD13	2.56	0.41
2:C:899:GLN:NE2	2:C:901:TYR:OH	2.54	0.41
2:C:905:ILE:C	2:C:907:ASP:H	2.29	0.41
3:D:1323:GLN:HA	3:D:1324:PRO:HD3	1.94	0.41
5:F:167:PRO:O	5:F:171:LYS:N	2.53	0.41
1:K:221:HIS:HA	1:K:224:TYR:CD2	2.56	0.41
1:L:216:GLU:OE1	1:L:219:ARG:NH2	2.42	0.41
2:M:172:ILE:HD11	2:M:261:ILE:HD11	2.03	0.41
3:N:262:LYS:HE2	3:N:341:GLU:OE2	2.21	0.41
3:N:293:VAL:HG22	3:N:296:GLU:HG3	2.03	0.41
3:N:879:ARG:HD3	3:N:902:LEU:O	2.21	0.41
5:P:134:LYS:HD3	5:P:134:LYS:HA	1.93	0.41
1:B:111:ALA:HB3	1:B:125:PRO:HA	2.03	0.41
2:C:704:HIS:CE1	2:C:1000:MET:HE1	2.56	0.41
3:D:1092:GLY:HA3	7:G:14:DA:O4'	2.21	0.41
1:K:64:GLU:HG2	1:K:76:VAL:HG22	2.03	0.41
1:K:101:LEU:HD21	1:K:109:VAL:HG11	2.03	0.41
2:M:1090:LYS:HA	2:M:1090:LYS:HD3	1.78	0.41
3:N:181:ASP:HB2	3:N:205:TYR:CD2	2.56	0.41
3:N:711:LEU:HD12	3:N:778:LEU:HD23	2.02	0.41
3:N:1323:GLN:HA	3:N:1324:PRO:HD3	1.93	0.41
4:O:40:LEU:HG	4:O:67:GLU:HG2	2.03	0.41
2:C:1052:MET:HE1	3:D:748:HIS:HB3	2.03	0.40
3:N:1151:ARG:HA	3:N:1151:ARG:HD3	1.95	0.40
1:A:54:THR:OG1	1:A:145:ASP:OD1	2.36	0.40
2:C:512:ARG:HB2	2:C:523:ILE:HD11	2.02	0.40
3:D:323:GLU:HB2	3:D:334:THR:HB	2.02	0.40
3:D:654:LYS:O	3:D:658:LEU:HG	2.21	0.40
5:F:172:ARG:O	5:F:176:ILE:HG12	2.21	0.40
1:K:20:TYR:OH	1:K:198:ARG:HD2	2.20	0.40
1:K:31:GLY:N	1:K:193:ASP:OD2	2.54	0.40
2:M:1019:GLN:HG2	2:M:1058:ASP:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:83:ASP:OD1	4:O:83:ASP:N	2.55	0.40
1:B:222:LEU:HD23	1:B:222:LEU:HA	1.96	0.40
2:C:983:ILE:HG21	2:C:987:ILE:HD11	2.02	0.40
4:E:80:VAL:HG21	4:E:85:LEU:HD13	2.02	0.40
5:F:285:GLU:HA	5:F:286:PRO:HD3	1.79	0.40
5:F:402:ASN:O	5:F:406:ARG:N	2.54	0.40
2:M:118:ILE:HG12	2:M:382:ILE:HD13	2.03	0.40
3:N:192:ALA:HB1	3:N:193:PRO:HD2	2.02	0.40
3:N:255:GLU:HG2	3:N:274:ARG:HH12	1.87	0.40
4:O:3:GLU:HA	4:O:4:PRO:HD3	1.93	0.40
6:S:16:DC:H2''	6:S:17:DA:H5'	2.04	0.40
1:B:57:TYR:CG	1:B:161:ARG:HD2	2.56	0.40
1:B:90:LEU:HD21	1:B:121:GLU:HB2	2.03	0.40
2:C:499:ALA:HB2	2:C:533:ASP:HB2	2.02	0.40
3:D:233:LYS:HB2	3:D:236:TYR:CZ	2.57	0.40
3:D:431:VAL:HG21	3:D:448:GLU:HG2	2.03	0.40
3:N:483:HIS:CE1	3:N:488:ARG:HD3	2.56	0.40
2:C:716:LYS:HE3	3:D:37:LEU:HG	2.03	0.40
2:C:775:ARG:HH11	2:C:782:ALA:HA	1.86	0.40
2:C:874:LEU:HD23	3:D:1023:MET:SD	2.62	0.40
3:D:150:ARG:HH22	3:D:468:LEU:HD21	1.85	0.40
3:D:619:LEU:HD11	3:D:1439:SER:HB2	2.04	0.40
2:M:263:ASP:O	2:M:267:TYR:N	2.53	0.40
2:M:872:ASN:HA	2:M:873:PRO:HD2	1.95	0.40
3:N:959:GLU:OE1	3:N:959:GLU:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [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	229/315 (73%)	224 (98%)	5 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	221/315 (70%)	216 (98%)	5 (2%)	0	100	100
1	K	229/315 (73%)	225 (98%)	4 (2%)	0	100	100
1	L	221/315 (70%)	217 (98%)	3 (1%)	1 (0%)	24	54
2	C	1108/1119 (99%)	1075 (97%)	33 (3%)	0	100	100
2	M	1109/1119 (99%)	1080 (97%)	29 (3%)	0	100	100
3	D	1482/1524 (97%)	1445 (98%)	37 (2%)	0	100	100
3	N	1482/1524 (97%)	1447 (98%)	35 (2%)	0	100	100
4	E	92/99 (93%)	90 (98%)	2 (2%)	0	100	100
4	O	92/99 (93%)	90 (98%)	2 (2%)	0	100	100
5	F	344/443 (78%)	334 (97%)	9 (3%)	1 (0%)	36	64
5	P	344/443 (78%)	339 (98%)	5 (2%)	0	100	100
All	All	6953/7630 (91%)	6782 (98%)	169 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains [i](#)

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%)	197 (98%)	3 (2%)	57	73
1	B	196/273 (72%)	194 (99%)	2 (1%)	68	77
1	K	200/273 (73%)	198 (99%)	2 (1%)	68	77
1	L	196/273 (72%)	194 (99%)	2 (1%)	68	77
2	C	936/941 (100%)	920 (98%)	16 (2%)	53	71
2	M	937/941 (100%)	918 (98%)	19 (2%)	48	69
3	D	1253/1279 (98%)	1221 (97%)	32 (3%)	40	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	N	1253/1279 (98%)	1226 (98%)	27 (2%)	45	68
4	E	82/88 (93%)	79 (96%)	3 (4%)	30	58
4	O	82/88 (93%)	81 (99%)	1 (1%)	63	75
5	F	301/388 (78%)	285 (95%)	16 (5%)	20	48
5	P	301/388 (78%)	296 (98%)	5 (2%)	53	71
All	All	5937/6484 (92%)	5809 (98%)	128 (2%)	45	68

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	112	ARG
1	A	142	VAL
1	B	90	LEU
1	B	115	LEU
2	C	34	VAL
2	C	118	ILE
2	C	182	VAL
2	C	217	LEU
2	C	240	THR
2	C	250	ARG
2	C	299	LYS
2	C	300	ASP
2	C	336	VAL
2	C	360	LEU
2	C	382	ILE
2	C	405	ARG
2	C	512	ARG
2	C	610	ARG
2	C	714	ASP
2	C	815	LEU
3	D	3	LYS
3	D	67	ARG
3	D	71	LYS
3	D	133	ILE
3	D	175	VAL
3	D	231	VAL
3	D	270	LEU
3	D	297	ILE
3	D	354	VAL

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Mol	Chain	Res	Type
3	D	452	ILE
3	D	632	VAL
3	D	709	HIS
3	D	741	ASP
3	D	754	PHE
3	D	778	LEU
3	D	810	GLU
3	D	894	LYS
3	D	904	VAL
3	D	971	LEU
3	D	986	ARG
3	D	1055	VAL
3	D	1067	VAL
3	D	1083	ASP
3	D	1129	THR
3	D	1137	ARG
3	D	1188	VAL
3	D	1252	ILE
3	D	1283	ILE
3	D	1286	THR
3	D	1290	LEU
3	D	1493	LYS
3	D	1501	GLU
4	E	73	LEU
4	E	84	ARG
4	E	87	LYS
5	F	88	ILE
5	F	95	THR
5	F	97	GLU
5	F	156	VAL
5	F	295	MET
5	F	358	LEU
5	F	360	LYS
5	F	365	GLU
5	F	383	LEU
5	F	392	VAL
5	F	395	GLU
5	F	399	GLN
5	F	407	LYS
5	F	408	LEU
5	F	409	LYS
5	F	414	ARG

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Mol	Chain	Res	Type
1	K	6	LEU
1	K	189	ARG
1	L	7	LYS
1	L	154	GLU
2	M	104	ASP
2	M	182	VAL
2	M	200	LEU
2	M	217	LEU
2	M	261	ILE
2	M	276	LYS
2	M	284	ARG
2	M	302	VAL
2	M	342	ASP
2	M	397	GLU
2	M	419	THR
2	M	513	VAL
2	M	583	LEU
2	M	617	ASP
2	M	670	GLN
2	M	775	ARG
2	M	807	ARG
2	M	1076	VAL
2	M	1105	LYS
3	N	4	GLU
3	N	67	ARG
3	N	71	LYS
3	N	231	VAL
3	N	255	GLU
3	N	272	LEU
3	N	273	ARG
3	N	346	ARG
3	N	354	VAL
3	N	415	VAL
3	N	448	GLU
3	N	452	ILE
3	N	632	VAL
3	N	633	VAL
3	N	687	VAL
3	N	709	HIS
3	N	754	PHE
3	N	778	LEU
3	N	810	GLU

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Mol	Chain	Res	Type
3	N	894	LYS
3	N	907	GLU
3	N	986	ARG
3	N	1067	VAL
3	N	1129	THR
3	N	1184	GLN
3	N	1267	ARG
3	N	1283	ILE
4	O	49	GLN
5	P	95	THR
5	P	262	VAL
5	P	295	MET
5	P	323	ASP
5	P	380	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	HIS
1	A	213	GLN
2	C	31	GLN
2	C	99	GLN
2	C	102	HIS
2	C	117	HIS
2	C	390	GLN
2	C	538	GLN
2	C	991	GLN
2	C	1026	GLN
2	C	1047	HIS
3	D	66	GLN
3	D	316	GLN
3	D	388	HIS
3	D	669	ASN
3	D	680	GLN
3	D	703	ASN
3	D	724	GLN
3	D	973	GLN
3	D	976	GLN
3	D	994	GLN
3	D	1033	GLN
3	D	1046	GLN
3	D	1172	HIS

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Mol	Chain	Res	Type
3	D	1184	GLN
4	E	49	GLN
5	F	83	GLN
5	F	170	HIS
5	F	411	HIS
2	M	219	GLN
2	M	498	GLN
2	M	538	GLN
2	M	683	ASN
2	M	1026	GLN
3	N	66	GLN
3	N	386	HIS
3	N	669	ASN
3	N	703	ASN
3	N	717	GLN
3	N	724	GLN
3	N	727	GLN
3	N	994	GLN
3	N	1033	GLN
3	N	1184	GLN
3	N	1254	GLN
3	N	1359	GLN
3	N	1374	GLN
4	O	49	GLN
5	P	83	GLN
5	P	185	GLN
5	P	402	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

Of 19 ligands modelled in this entry, 13 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	DPO	N	1605	8	6,8,8	1.02	0	12,13,13	0.78	0
10	C5P	N	1604	8,12	18,21,22	0.28	0	25,30,33	0.36	0
10	C5P	D	2005	8,12	18,21,22	0.30	0	25,30,33	0.36	0
12	COD	R	101	10	28,29,46	1.65	6 (21%)	43,45,68	1.32	4 (9%)
12	COD	G	101	10	30,30,46	1.59	6 (20%)	43,46,68	1.33	4 (9%)
11	DPO	D	2006	8	6,8,8	0.99	0	12,13,13	0.89	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	DPO	N	1605	8	-	0/6/6/6	-
10	C5P	N	1604	8,12	-	0/7/25/26	0/2/2/2
10	C5P	D	2005	8,12	-	2/7/25/26	0/2/2/2
12	COD	R	101	10	-	6/16/32/59	0/3/3/3
12	COD	G	101	10	-	3/19/35/59	0/3/3/3
11	DPO	D	2006	8	-	0/6/6/6	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	R	101	COD	C6-N7	3.76	1.43	1.34
12	G	101	COD	C6-N7	3.75	1.43	1.34
12	R	101	COD	C18-C16	3.21	1.61	1.51
12	G	101	COD	C2-N3	3.21	1.39	1.33
12	G	101	COD	C18-C16	3.16	1.61	1.51
12	R	101	COD	C2-N3	3.08	1.39	1.33
12	R	101	COD	C2-N1	2.81	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	G	101	COD	C2-N1	2.78	1.38	1.33
12	G	101	COD	C4-N10	2.74	1.43	1.37
12	R	101	COD	C4-N10	2.55	1.43	1.37
12	R	101	COD	O13-C12	-2.25	1.37	1.43
12	G	101	COD	O13-C12	-2.22	1.37	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	R	101	COD	N3-C2-N1	-5.29	120.57	128.58
12	G	101	COD	N3-C2-N1	-5.26	120.61	128.58
12	G	101	COD	C14-C12-C11	3.39	107.87	101.46
12	R	101	COD	C14-C12-C11	2.72	106.61	101.46
12	G	101	COD	O17-C16-C18	2.24	116.52	109.33
12	R	101	COD	C2-N1-C6	2.20	122.34	118.73
12	R	101	COD	O17-C16-C18	2.10	116.05	109.33
12	G	101	COD	C2-N1-C6	2.05	122.09	118.73

There are no chirality outliers.

All (11) torsion outliers are listed below:

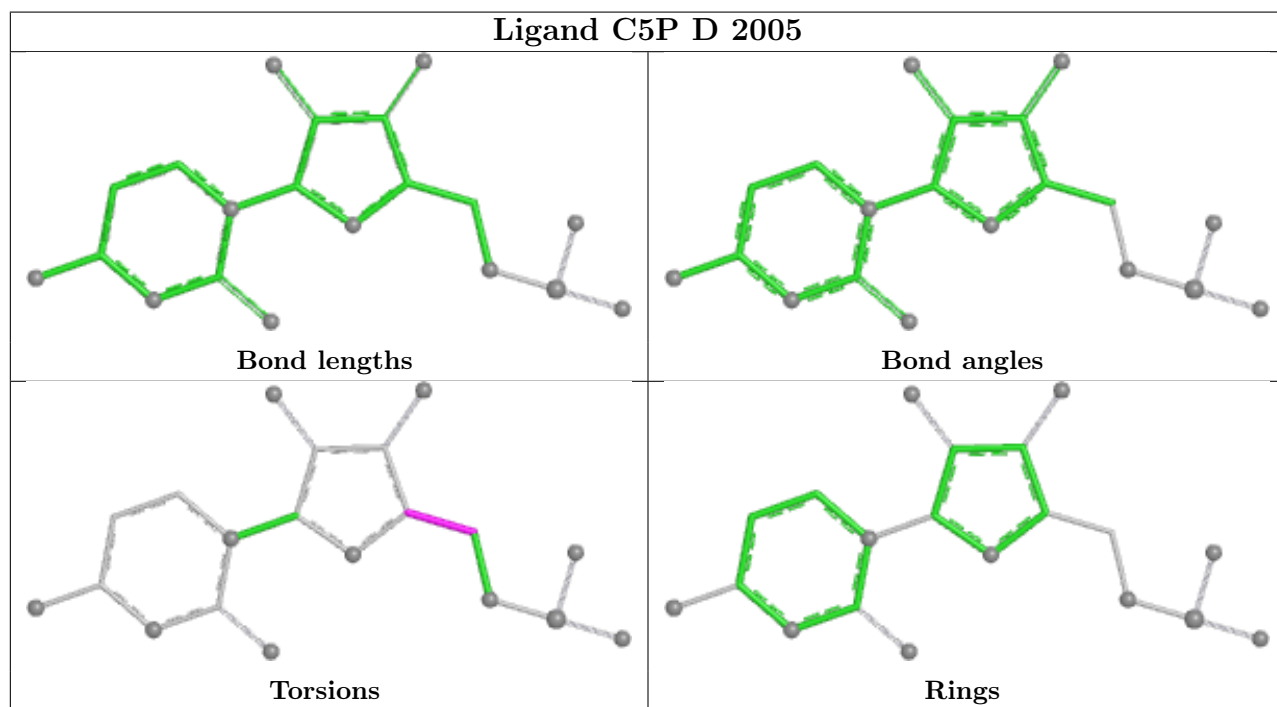
Mol	Chain	Res	Type	Atoms
10	D	2005	C5P	O4'-C4'-C5'-O5'
12	R	101	COD	C18-O19-P20-O21
12	R	101	COD	C18-O19-P20-O22
12	R	101	COD	C18-O19-P20-O23
10	D	2005	C5P	C3'-C4'-C5'-O5'
12	R	101	COD	O17-C16-C18-O19
12	R	101	COD	C14-C16-C18-O19
12	G	101	COD	P20-O23-P24-O27
12	R	101	COD	P24-O23-P20-O22
12	G	101	COD	P20-O23-P24-O26
12	G	101	COD	P24-O23-P20-O21

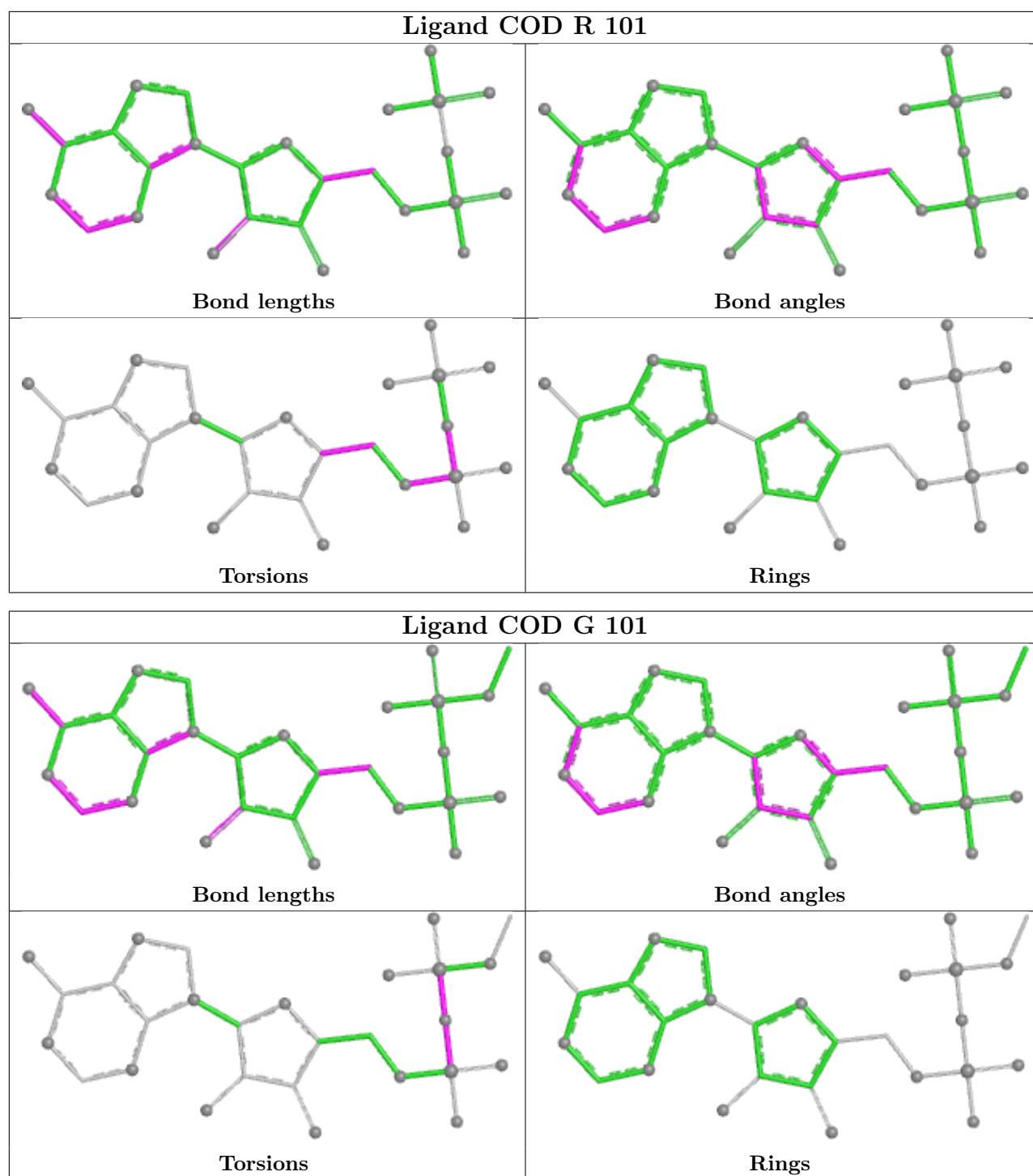
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	N	1604	C5P	3	0
10	D	2005	C5P	1	0

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





5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data i

6.1 Protein, DNA and RNA chains i

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%)	0.24	7 (3%) 52 30	29, 51, 78, 126	1 (0%)
1	B	223/315 (70%)	0.08	0 100 100	26, 53, 93, 122	0
1	K	231/315 (73%)	-0.10	3 (1%) 75 53	22, 38, 65, 128	1 (0%)
1	L	223/315 (70%)	-0.00	1 (0%) 88 75	21, 49, 82, 102	0
2	C	1112/1119 (99%)	0.59	94 (8%) 16 9	12, 58, 115, 132	3 (0%)
2	M	1112/1119 (99%)	-0.20	8 (0%) 84 66	5, 32, 82, 118	4 (0%)
3	D	1486/1524 (97%)	0.05	28 (1%) 66 44	7, 43, 96, 131	4 (0%)
3	N	1486/1524 (97%)	-0.19	8 (0%) 87 72	4, 34, 85, 125	4 (0%)
4	E	94/99 (94%)	0.03	0 100 100	22, 44, 88, 102	0
4	O	94/99 (94%)	-0.17	0 100 100	14, 31, 67, 85	0
5	F	346/443 (78%)	0.75	33 (9%) 14 7	33, 70, 134, 152	0
5	P	346/443 (78%)	-0.04	0 100 100	14, 43, 93, 112	0
6	H	21/27 (77%)	0.85	1 (4%) 35 18	47, 92, 134, 155	0
6	S	21/27 (77%)	0.42	1 (4%) 35 18	35, 73, 118, 146	0
7	G	16/19 (84%)	0.72	1 (6%) 26 13	49, 77, 129, 134	0
7	R	16/19 (84%)	0.31	0 100 100	31, 60, 131, 137	0
All	All	7058/7722 (91%)	0.08	185 (2%) 57 34	4, 44, 99, 155	17 (0%)

All (185) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	63	GLY	8.3
2	C	200	LEU	5.6
2	C	196	LEU	5.6
2	C	807	ARG	5.5
2	C	48	PHE	5.4

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Mol	Chain	Res	Type	RSRZ
5	F	386	VAL	5.1
2	C	68	PHE	5.0
3	D	674	ARG	5.0
2	C	66	LEU	5.0
2	M	102	HIS	4.4
2	C	769	PRO	4.4
2	C	102	HIS	4.2
2	C	591	SER	4.1
1	A	139	ASN	4.0
2	C	52	PHE	4.0
5	F	383	LEU	3.9
5	F	368	VAL	3.9
1	A	233	VAL	3.8
2	C	65	VAL	3.8
2	C	302	VAL	3.8
2	C	101	ILE	3.7
2	C	236	ILE	3.7
2	C	146	VAL	3.6
3	N	1045	MET	3.6
3	D	191	LEU	3.6
2	C	272	ALA	3.5
1	K	139	ASN	3.5
2	C	258	TYR	3.4
5	F	378	GLY	3.4
2	C	268	ASP	3.4
3	D	1053	PHE	3.4
3	N	1053	PHE	3.4
2	M	64	LEU	3.3
1	K	233	VAL	3.3
5	F	142	ARG	3.3
2	M	807	ARG	3.2
2	C	1084	SER	3.2
2	C	221	LEU	3.2
2	C	194	VAL	3.2
5	F	397	ILE	3.2
2	C	100	LEU	3.2
5	F	390	PHE	3.2
2	C	638	ASP	3.2
5	F	366	ALA	3.2
5	F	404	ALA	3.2
2	C	199	VAL	3.2
1	K	232	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
2	C	64	LEU	3.1
2	C	367	LEU	3.1
2	C	396	ASP	3.1
3	D	184	GLU	3.1
3	D	412	GLY	3.1
2	C	461	VAL	3.0
3	N	184	GLU	3.0
5	F	325	LYS	3.0
5	F	392	VAL	3.0
3	D	1045	MET	3.0
5	F	395	GLU	3.0
5	F	139	ALA	3.0
3	D	423	ASP	3.0
2	C	378	LEU	2.9
3	D	226	PRO	2.9
2	C	344	PHE	2.9
6	H	11	DG	2.8
3	N	674	ARG	2.8
2	C	108	ILE	2.8
2	C	191	PHE	2.8
5	F	411	HIS	2.8
2	C	369	PRO	2.8
3	N	1128	VAL	2.8
2	C	260	LEU	2.8
5	F	358	LEU	2.8
5	F	408	LEU	2.8
2	C	259	GLY	2.7
3	D	352	ASN	2.7
5	F	141	VAL	2.7
5	F	369	LEU	2.7
2	C	176	VAL	2.7
5	F	422	LEU	2.7
5	F	389	PHE	2.7
2	M	365	ASP	2.7
5	F	410	TYR	2.7
2	C	373	VAL	2.7
2	C	347	GLY	2.6
5	F	391	GLY	2.6
2	C	235	LEU	2.6
2	C	207	LEU	2.6
2	C	777	ILE	2.6
3	D	1128	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
2	C	270	GLY	2.5
2	C	357	GLU	2.5
3	D	311	LEU	2.5
2	C	287	GLY	2.5
2	C	303	PHE	2.5
3	D	193	PRO	2.5
3	D	68	PHE	2.5
2	C	269	LEU	2.5
2	C	362	GLY	2.5
3	N	1499	ARG	2.4
2	C	105	THR	2.4
2	C	247	PRO	2.4
2	C	106	GLY	2.4
7	G	4	DT	2.4
2	C	775	ARG	2.4
5	F	364	ARG	2.4
2	M	97	ARG	2.4
2	C	107	LEU	2.4
3	D	211	VAL	2.4
5	F	403	LYS	2.4
3	D	680	GLN	2.4
2	M	107	LEU	2.4
5	F	190	ALA	2.3
3	D	316	GLN	2.3
5	F	407	LYS	2.3
2	M	629	TYR	2.3
2	C	526	PRO	2.3
2	C	593	ALA	2.3
2	C	98	LEU	2.3
2	C	806	LEU	2.3
3	N	368	VAL	2.3
1	L	228	PRO	2.3
1	A	130	ALA	2.3
2	C	340	MET	2.3
2	C	372	LEU	2.3
2	C	188	LYS	2.3
2	C	767	PRO	2.3
5	F	405	LEU	2.3
3	D	432	TYR	2.3
5	F	357	ALA	2.2
1	A	131	THR	2.2
2	C	813	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
2	C	745	ILE	2.2
1	A	232	ALA	2.2
2	C	998	TYR	2.2
2	C	41	ASN	2.2
2	C	213	ALA	2.2
2	C	741	GLY	2.2
2	C	114	PHE	2.2
2	C	261	ILE	2.2
2	C	184	MET	2.2
2	C	360	LEU	2.2
2	C	352	ALA	2.2
2	M	361	MET	2.2
5	F	275	ALA	2.2
2	C	54	ILE	2.2
3	D	367	ILE	2.2
3	N	1275	SER	2.2
2	C	770	GLU	2.2
3	D	55	ASP	2.2
2	C	257	VAL	2.1
3	D	196	VAL	2.1
5	F	399	GLN	2.1
5	F	306	GLU	2.1
2	C	67	ASP	2.1
6	S	25	DA	2.1
5	F	414	ARG	2.1
2	C	201	GLY	2.1
2	C	113	VAL	2.1
2	C	195	LEU	2.1
5	F	376	ILE	2.1
2	C	115	LEU	2.1
2	C	251	ASP	2.1
2	C	810	ASP	2.1
3	D	142	LEU	2.1
2	C	291	ALA	2.1
2	C	281	LEU	2.1
2	C	815	LEU	2.1
3	D	393	ILE	2.1
1	A	70	GLY	2.1
2	C	273	GLY	2.1
2	C	271	GLU	2.1
3	D	266	GLU	2.1
2	C	51	THR	2.0

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Mol	Chain	Res	Type	RSRZ
2	C	255	ALA	2.0
3	D	345	TYR	2.0
2	C	264	PRO	2.0
2	C	421	GLU	2.0
3	D	400	VAL	2.0
2	C	464	LEU	2.0
2	C	765	SER	2.0
3	D	307	ALA	2.0
3	D	173	PRO	2.0
2	C	34	VAL	2.0
3	D	264	LEU	2.0
1	A	129	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.

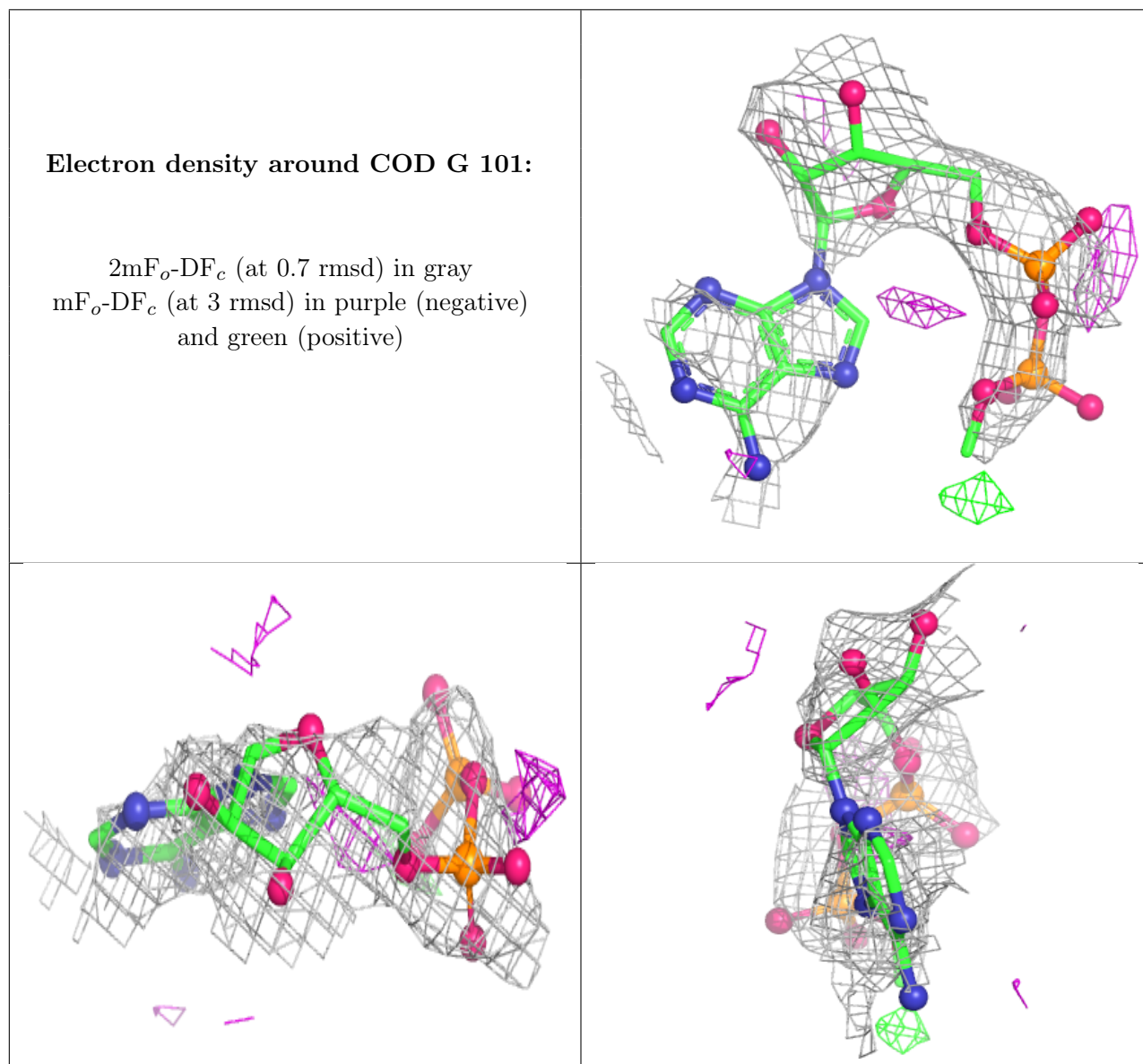
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
12	COD	G	101	28/44	0.64	0.17	50,73,102,116	28
8	MG	F	2001	1/1	0.71	0.09	92,92,92,92	0
10	C5P	D	2005	20/21	0.80	0.16	43,61,71,80	20
8	MG	B	2001	1/1	0.85	0.10	71,71,71,71	0
10	C5P	N	1604	20/21	0.86	0.15	24,34,49,57	20
11	DPO	D	2006	9/9	0.86	0.07	45,68,84,98	0
8	MG	D	2004	1/1	0.86	0.32	27,27,27,27	0
12	COD	R	101	27/44	0.86	0.13	35,43,62,65	27
11	DPO	N	1605	9/9	0.87	0.08	26,51,74,84	0
8	MG	L	1601	1/1	0.88	0.28	25,25,25,25	0
8	MG	N	1606	1/1	0.88	0.07	36,36,36,36	0

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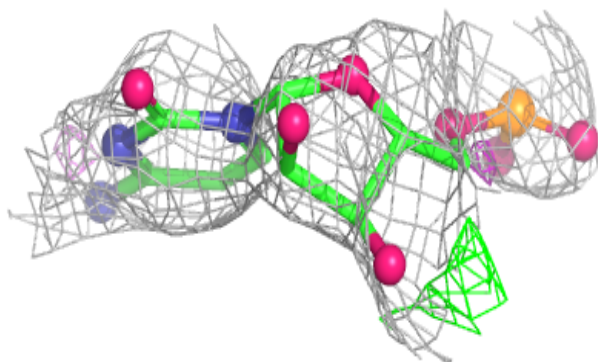
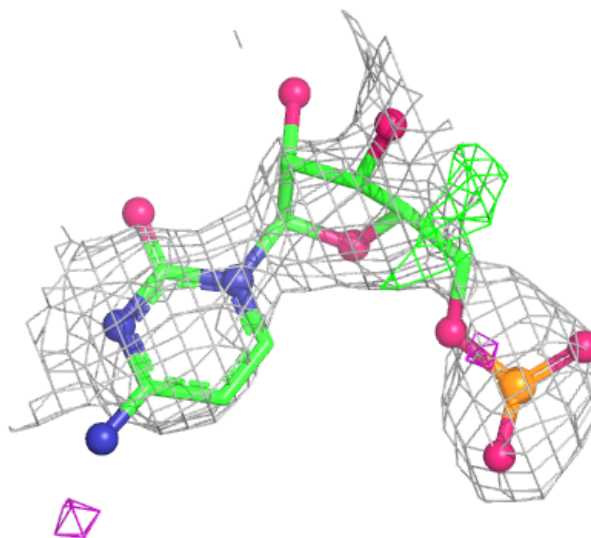
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	MG	P	2001	1/1	0.90	0.06	38,38,38,38	0
8	MG	D	2007	1/1	0.91	0.06	49,49,49,49	0
9	ZN	D	2002	1/1	0.97	0.06	92,92,92,92	0
8	MG	N	1603	1/1	0.98	0.06	13,13,13,13	0
8	MG	D	2003	1/1	0.98	0.04	22,22,22,22	0
9	ZN	D	2001	1/1	1.00	0.02	20,20,20,20	0
9	ZN	N	1601	1/1	1.00	0.02	16,16,16,16	0
9	ZN	N	1602	1/1	1.00	0.02	50,50,50,50	0

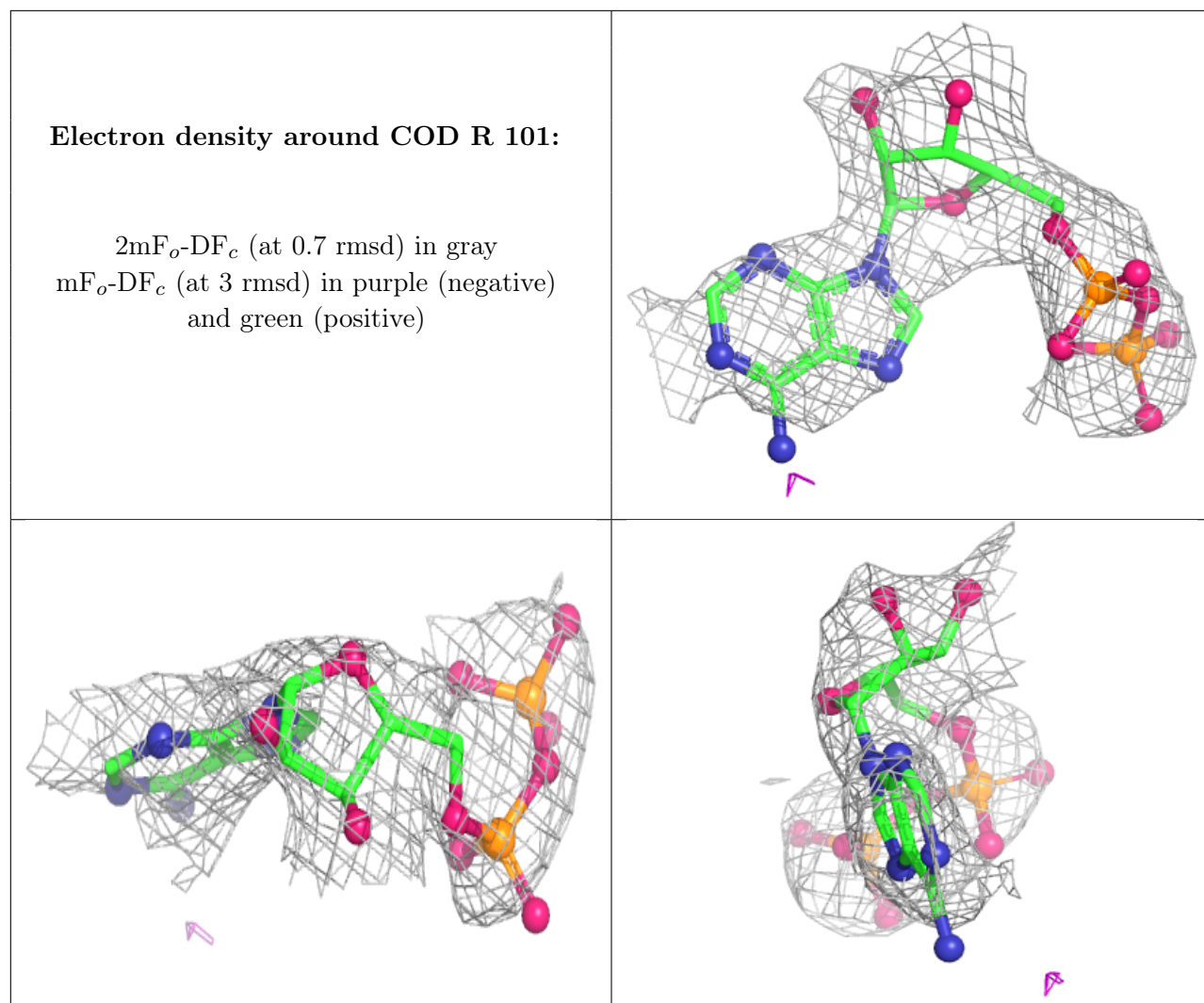
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



Electron density around C5P D 2005:

$2mF_o-DF_c$ (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.