Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:50 PM GMT

PDB ID	:	4G7H
Title	:	Crystal structure of Thermus thermophilus transcription initiation complex
Authors	:	Zhang, Y.; Ebright, R.H.
Deposited on	:	2012-07-20
Resolution	:	2.90 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

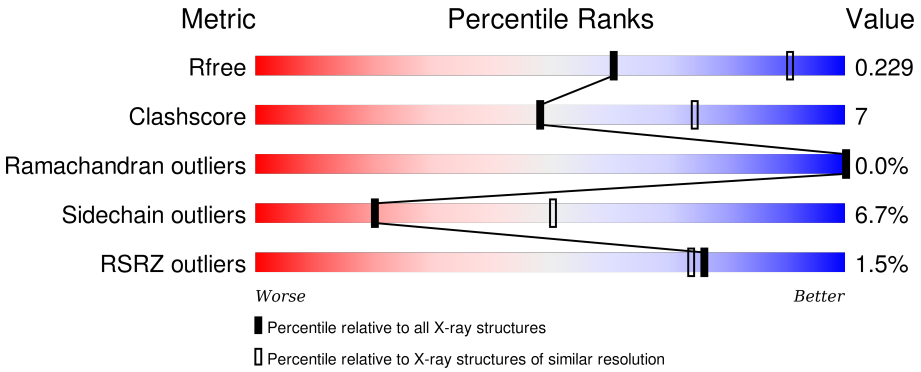
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.90 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}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	54% 15% • 28%
1	B	315	% 57% 11% • 30%
1	K	315	53% 17% • 28%
1	L	315	% 59% 11% • 29%
2	C	1119	% 77% 20% ••

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Mol	Chain	Length	Quality of chain
2	M	1119	3% 77% 20%
3	D	1524	% 79% 17%
3	N	1524	2% 78% 17%
4	E	99	79% 16% 5%
4	O	99	77% 18% 5%
5	F	443	63% 15% 22%
5	P	443	2% 58% 16% 22%
6	G	19	68% 16% 16%
6	Q	19	63% 21% 16%
7	H	27	33% 44% 11% 11%
7	R	27	44% 37% 7% 11%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	MG	B	2001	-	-	-	X
8	MG	D	2004	-	-	-	X
8	MG	K	1001	-	-	-	X
8	MG	N	2004	-	-	-	X
9	ZN	D	2001	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 57420 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	226	Total	C	N	O	S	0	0	0
			1782	1138	310	332	2			
1	B	222	Total	C	N	O	S	0	0	0
			1750	1118	304	326	2			
1	K	226	Total	C	N	O	S	0	0	0
			1782	1138	310	332	2			
1	L	225	Total	C	N	O	S	0	0	0
			1773	1133	308	330	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1111	Total	C	N	O	S	0	0	0
			8770	5548	1564	1634	24			
2	M	1111	Total	C	N	O	S	0	0	0
			8770	5548	1564	1634	24			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	94	Total	C	N	O	S	0	0	0
			761	486	132	139	4			
4	O	94	Total	C	N	O	S	0	0	0
			761	486	132	139	4			

- Molecule 5 is a protein called RNA polymerase sigma factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	346	Total	C	N	O	S	0	0	0
			2807	1770	509	524	4			
5	P	347	Total	C	N	O	S	0	0	0
			2814	1774	510	526	4			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-19	MET	-	EXPRESSION TAG	UNP Q5SKW1
F	-18	GLY	-	EXPRESSION TAG	UNP Q5SKW1
F	-17	SER	-	EXPRESSION TAG	UNP Q5SKW1
F	-16	SER	-	EXPRESSION TAG	UNP Q5SKW1
F	-15	HIS	-	EXPRESSION TAG	UNP Q5SKW1
F	-14	HIS	-	EXPRESSION TAG	UNP Q5SKW1
F	-13	HIS	-	EXPRESSION TAG	UNP Q5SKW1
F	-12	HIS	-	EXPRESSION TAG	UNP Q5SKW1
F	-11	HIS	-	EXPRESSION TAG	UNP Q5SKW1
F	-10	HIS	-	EXPRESSION TAG	UNP Q5SKW1
F	-9	SER	-	EXPRESSION TAG	UNP Q5SKW1
F	-8	SER	-	EXPRESSION TAG	UNP Q5SKW1
F	-7	GLY	-	EXPRESSION TAG	UNP Q5SKW1
F	-6	LEU	-	EXPRESSION TAG	UNP Q5SKW1
F	-5	VAL	-	EXPRESSION TAG	UNP Q5SKW1
F	-4	PRO	-	EXPRESSION TAG	UNP Q5SKW1
F	-3	ARG	-	EXPRESSION TAG	UNP Q5SKW1
F	-2	GLY	-	EXPRESSION TAG	UNP Q5SKW1
F	-1	SER	-	EXPRESSION TAG	UNP Q5SKW1
F	0	HIS	-	EXPRESSION TAG	UNP Q5SKW1
P	-19	MET	-	EXPRESSION TAG	UNP Q5SKW1
P	-18	GLY	-	EXPRESSION TAG	UNP Q5SKW1
P	-17	SER	-	EXPRESSION TAG	UNP Q5SKW1
P	-16	SER	-	EXPRESSION TAG	UNP Q5SKW1
P	-15	HIS	-	EXPRESSION TAG	UNP Q5SKW1
P	-14	HIS	-	EXPRESSION TAG	UNP Q5SKW1
P	-13	HIS	-	EXPRESSION TAG	UNP Q5SKW1
P	-12	HIS	-	EXPRESSION TAG	UNP Q5SKW1
P	-11	HIS	-	EXPRESSION TAG	UNP Q5SKW1
P	-10	HIS	-	EXPRESSION TAG	UNP Q5SKW1
P	-9	SER	-	EXPRESSION TAG	UNP Q5SKW1
P	-8	SER	-	EXPRESSION TAG	UNP Q5SKW1
P	-7	GLY	-	EXPRESSION TAG	UNP Q5SKW1
P	-6	LEU	-	EXPRESSION TAG	UNP Q5SKW1

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Chain	Residue	Modelled	Actual	Comment	Reference
P	-5	VAL	-	EXPRESSION TAG	UNP Q5SKW1
P	-4	PRO	-	EXPRESSION TAG	UNP Q5SKW1
P	-3	ARG	-	EXPRESSION TAG	UNP Q5SKW1
P	-2	GLY	-	EXPRESSION TAG	UNP Q5SKW1
P	-1	SER	-	EXPRESSION TAG	UNP Q5SKW1
P	0	HIS	-	EXPRESSION TAG	UNP Q5SKW1

- Molecule 6 is a DNA chain called 5'-D(*CP*CP*T*GP*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*TP*CP*GP*AP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	16	Total	C	N	O	P	0	0	0
			328	156	63	94	15			
6	Q	16	Total	C	N	O	P	0	0	0
			328	156	63	94	15			

- Molecule 7 is a DNA chain called 5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*AP*GP*CP*TP*GP*TP*CP*AP*CP*GP*GP*AP*TP*GP*CP*AP*GP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	24	Total	C	N	O	P	0	0	0
			495	236	94	142	23			
7	R	24	Total	C	N	O	P	0	0	0
			495	236	94	142	23			

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

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

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

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

- Molecule 10 is water.

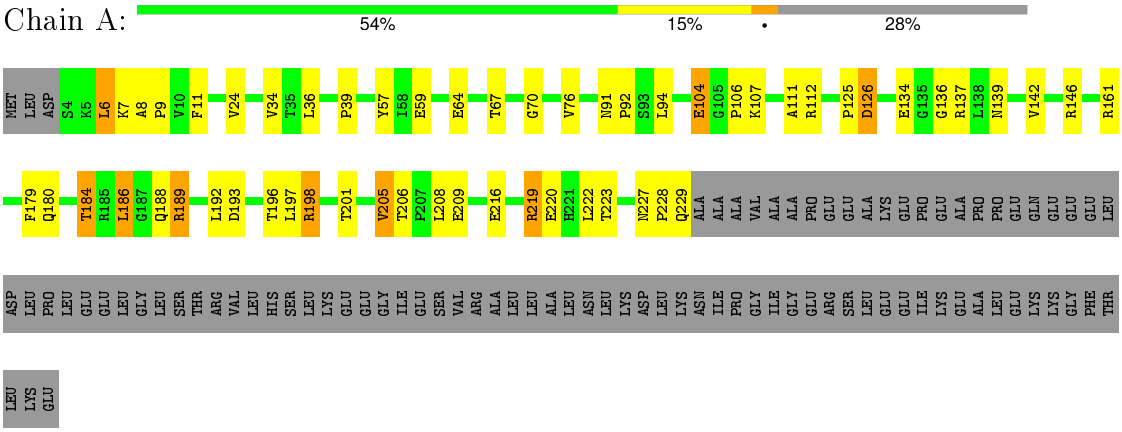
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	16	Total O 16 16	0	0
10	B	4	Total O 4 4	0	0
10	C	104	Total O 104 104	0	0
10	D	138	Total O 138 138	0	0
10	E	5	Total O 5 5	0	0
10	F	32	Total O 32 32	0	0
10	G	7	Total O 7 7	0	0
10	H	6	Total O 6 6	0	0
10	K	12	Total O 12 12	0	0
10	L	8	Total O 8 8	0	0
10	M	58	Total O 58 58	0	0
10	N	89	Total O 89 89	0	0
10	O	6	Total O 6 6	0	0
10	P	21	Total O 21 21	0	0
10	Q	3	Total O 3 3	0	0
10	R	5	Total O 5 5	0	0

3 Residue-property plots (i)

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

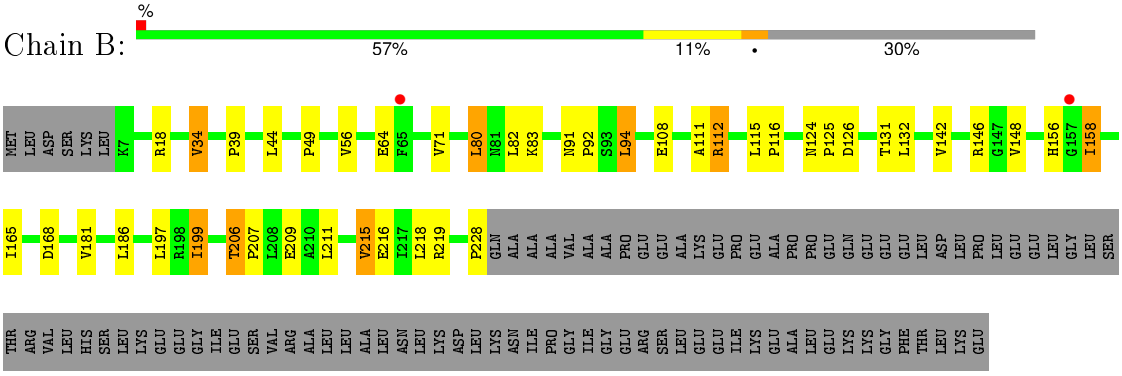
- Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:



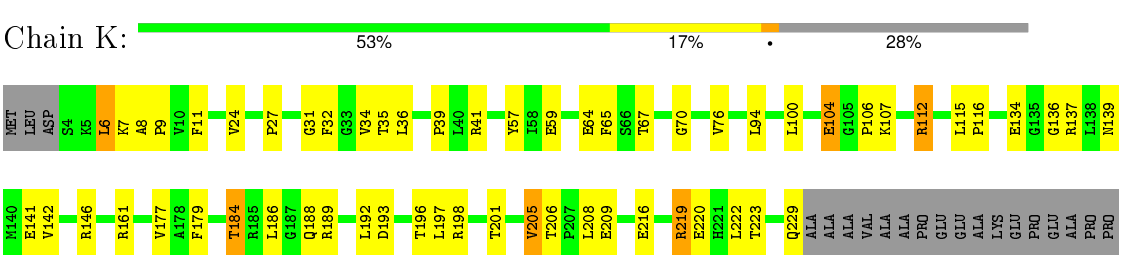
- Molecule 1: DNA-directed RNA polymerase subunit alpha

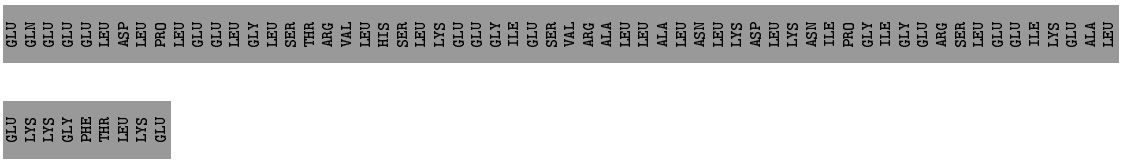
Chain B:



- Molecule 1: DNA-directed RNA polymerase subunit alpha

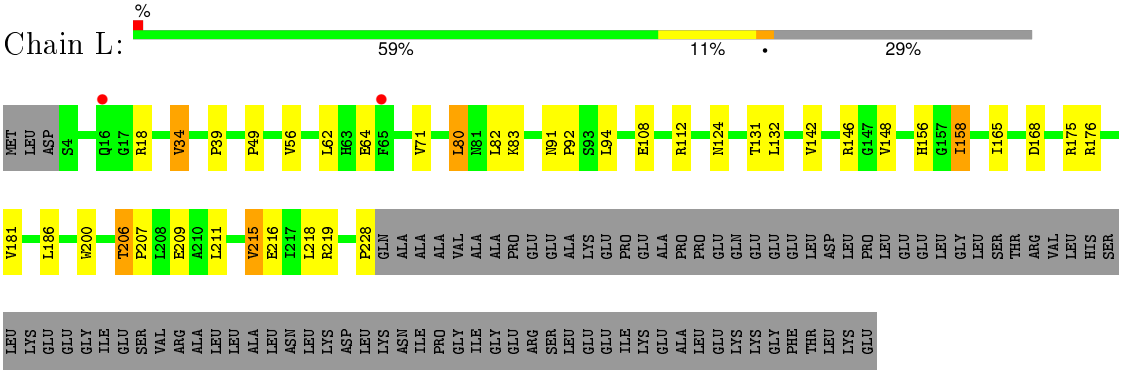
Chain K:





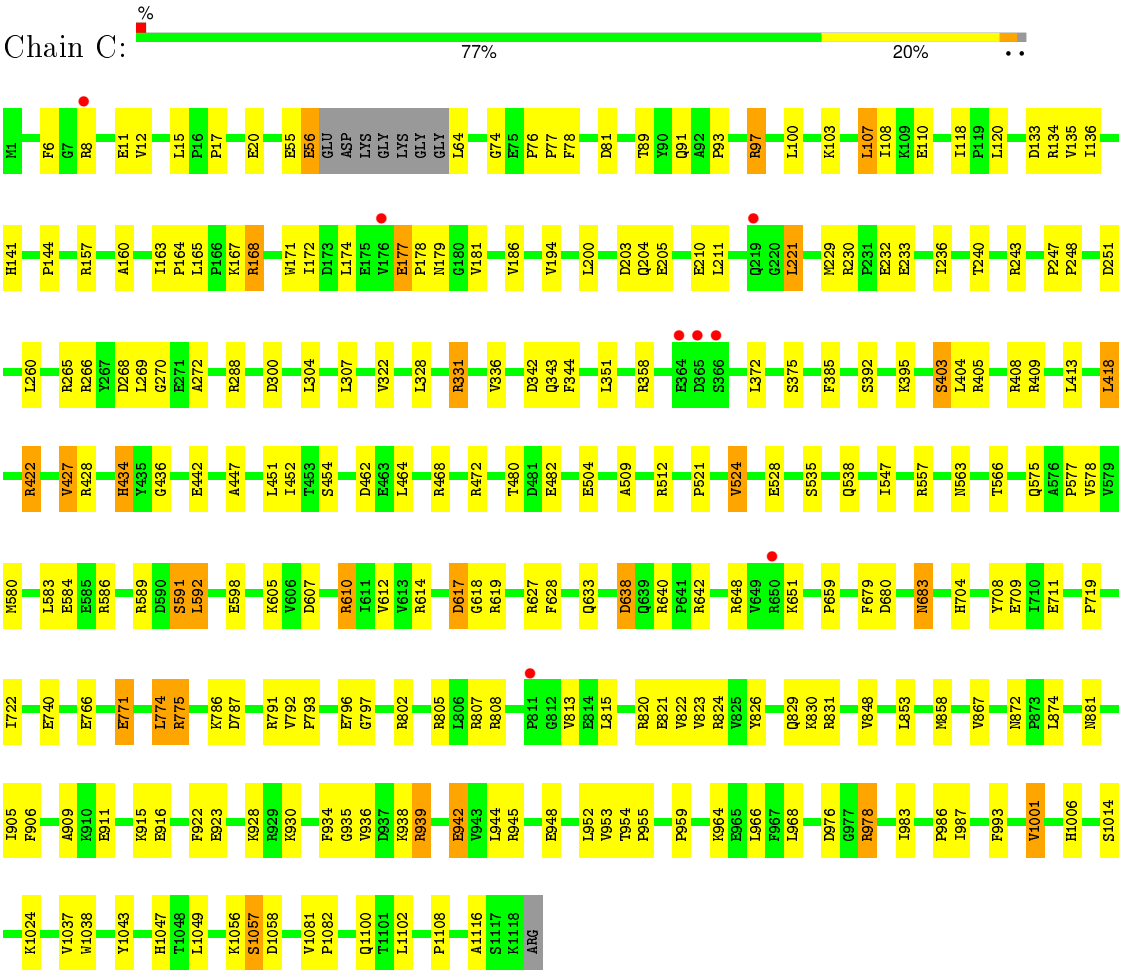
- Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain L:



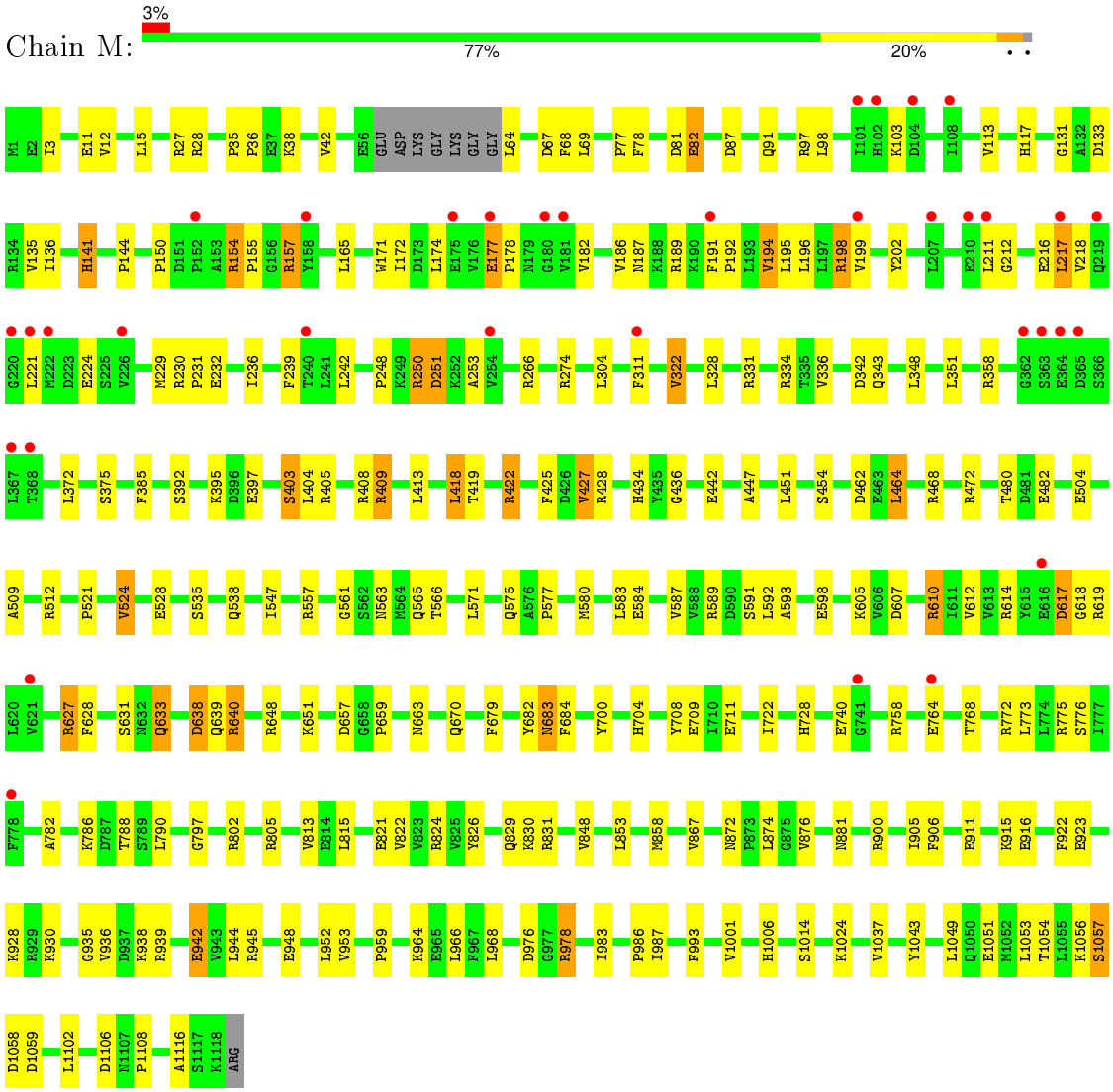
- Molecule 2: DNA-directed RNA polymerase subunit beta

Chain C:



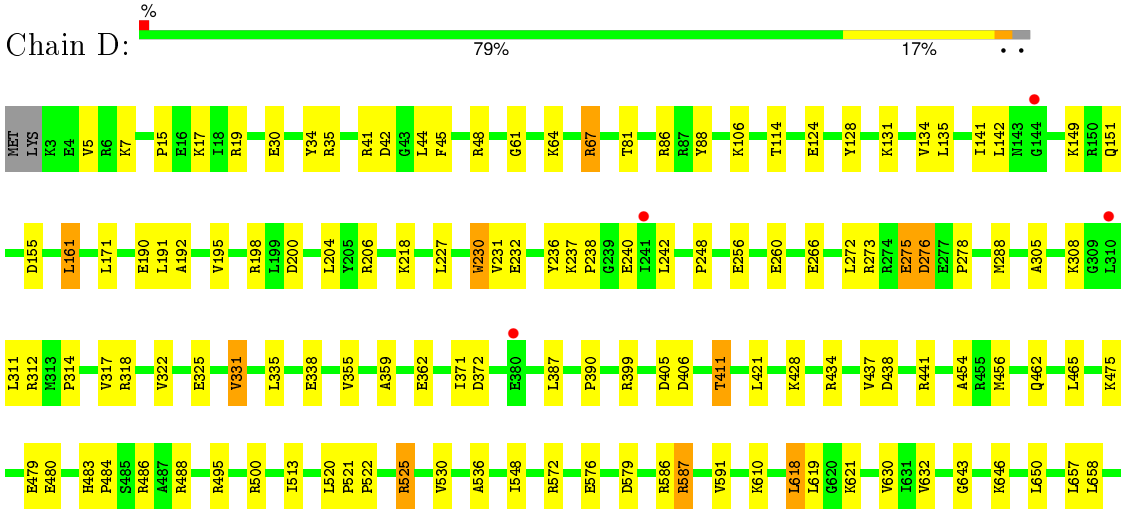
- Molecule 2: DNA-directed RNA polymerase subunit beta

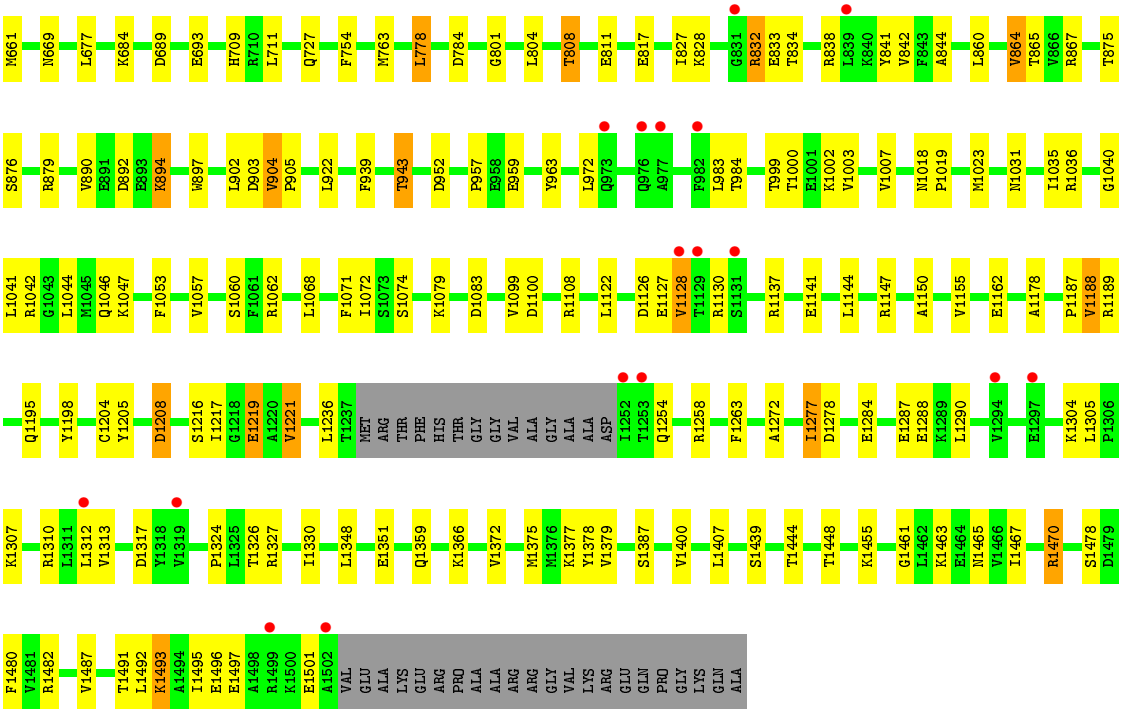
Chain M:



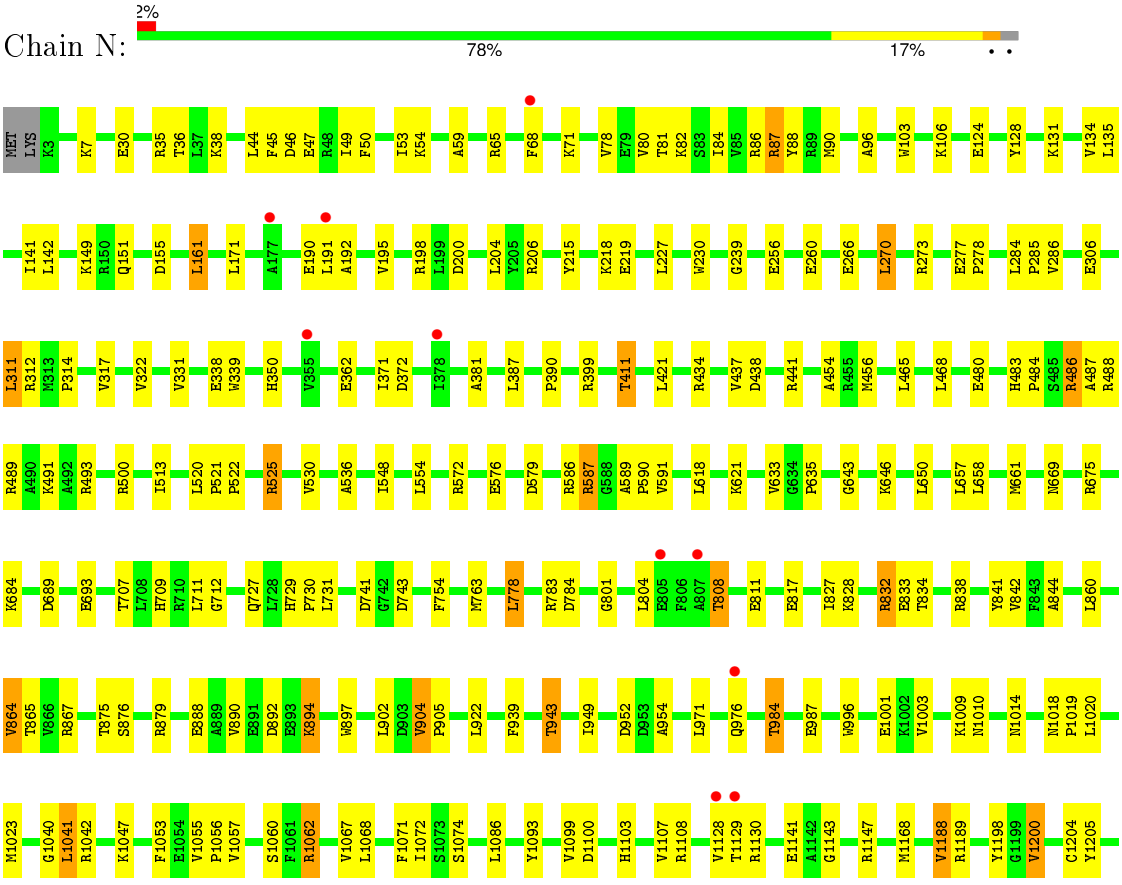
- Molecule 3: DNA-directed RNA polymerase subunit beta'

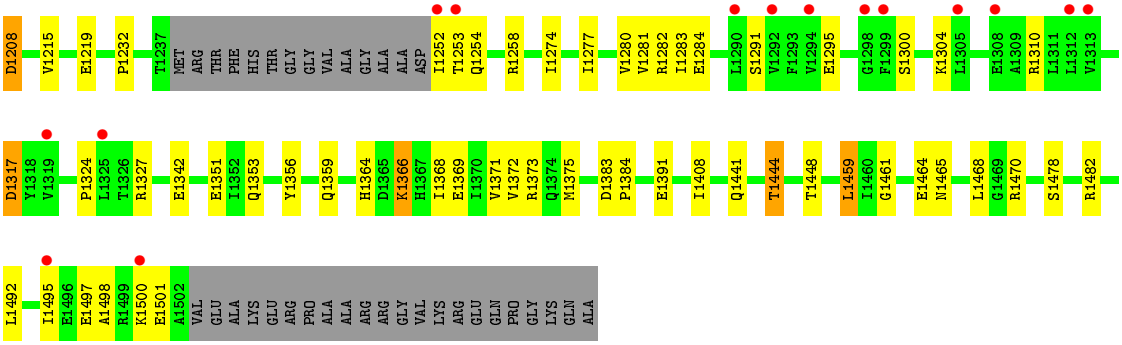
Chain D:





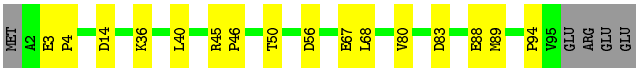
• Molecule 3: DNA-directed RNA polymerase subunit beta'





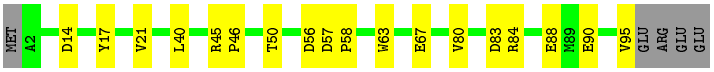
- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E:



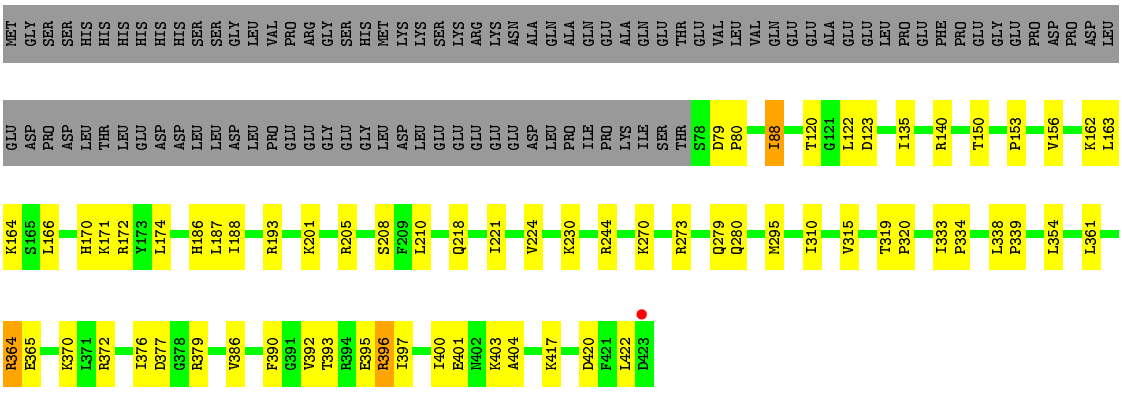
- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain O:



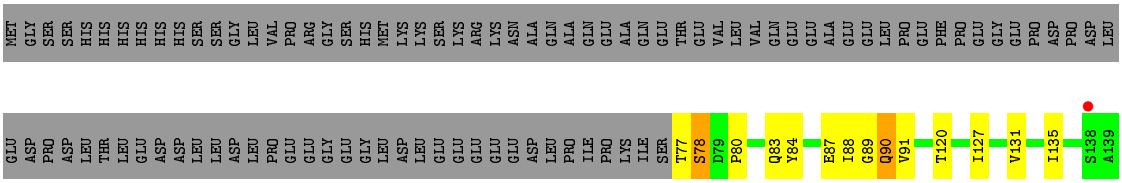
- Molecule 5: RNA polymerase sigma factor

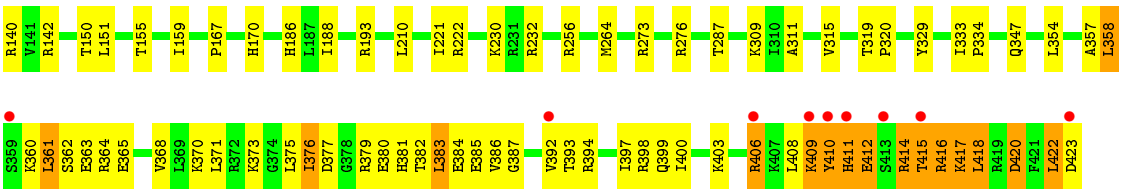
Chain F:



- Molecule 5: RNA polymerase sigma factor

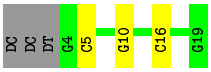
Chain P:





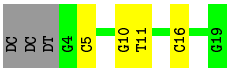
• Molecule 6: 5'-D(*CP*CP*T*GP*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*TP*CP*GP*AP*G)-3'

Chain G:



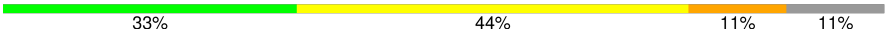
• Molecule 6: 5'-D(*CP*CP*T*GP*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*TP*CP*GP*AP*G)-3'

Chain Q:



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

Chain H:



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

Chain R:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	185.56Å 104.57Å 297.55Å 90.00° 98.32° 90.00°	Depositor
Resolution (Å)	49.27 – 2.90 49.90 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.27-2.90) 99.6 (49.90-2.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.11 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.188 , 0.226 0.191 , 0.229	Depositor DCC
R_{free} test set	2191 reflections (0.88%)	DCC
Wilson B-factor (Å^2)	61.5	Xtriage
Anisotropy	0.653	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 46.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	3 of 249334 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	57420	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.73 % 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 3.0020e-03.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: ZN, 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	0.32	0/1814	0.59	2/2466 (0.1%)
1	B	0.30	0/1782	0.52	0/2424
1	K	0.29	0/1814	0.67	5/2466 (0.2%)
1	L	0.29	0/1805	0.63	3/2454 (0.1%)
2	C	0.33	0/8937	0.54	4/12087 (0.0%)
2	M	0.32	0/8937	0.54	3/12087 (0.0%)
3	D	0.32	0/11944	0.50	0/16149
3	N	0.31	0/11944	0.50	1/16149 (0.0%)
4	E	0.28	0/775	0.45	0/1045
4	O	0.30	0/775	0.44	0/1045
5	F	0.30	0/2852	0.47	0/3837
5	P	0.30	0/2859	0.50	0/3847
6	G	0.60	0/368	1.26	3/567 (0.5%)
6	Q	0.54	0/368	1.27	4/567 (0.7%)
7	H	0.59	0/556	1.33	6/858 (0.7%)
7	R	0.58	0/556	1.35	7/858 (0.8%)
All	All	0.33	0/58086	0.57	38/78906 (0.0%)

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	422	ARG	NE-CZ-NH2	-13.77	113.42	120.30
2	M	422	ARG	NE-CZ-NH1	13.31	126.95	120.30
1	L	112	ARG	NE-CZ-NH1	-12.08	114.26	120.30
2	C	422	ARG	NE-CZ-NH1	-11.95	114.33	120.30
1	L	112	ARG	NE-CZ-NH2	11.77	126.19	120.30
1	K	112	ARG	NE-CZ-NH2	-11.61	114.50	120.30
2	C	422	ARG	NE-CZ-NH2	11.47	126.04	120.30
6	G	5	DC	O4'-C4'-C3'	-10.84	99.49	106.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	112	ARG	NE-CZ-NH1	10.80	125.70	120.30
1	K	198	ARG	NE-CZ-NH2	-10.79	114.90	120.30
1	A	198	ARG	NE-CZ-NH1	-10.70	114.95	120.30
6	Q	5	DC	O4'-C4'-C3'	-10.66	99.60	106.00
1	K	198	ARG	NE-CZ-NH1	9.81	125.21	120.30
1	A	198	ARG	NE-CZ-NH2	9.46	125.03	120.30
2	M	422	ARG	CD-NE-CZ	7.83	134.57	123.60
6	G	16	DC	O4'-C4'-C3'	-7.06	101.67	104.50
6	G	5	DC	C4'-C3'-C2'	-6.62	97.14	103.10
6	Q	5	DC	C4'-C3'-C2'	-6.57	97.18	103.10
2	C	422	ARG	CD-NE-CZ	6.42	132.59	123.60
7	R	23	DG	C4'-C3'-C2'	-6.38	97.36	103.10
7	H	23	DG	C4'-C3'-C2'	-6.34	97.39	103.10
7	R	16	DC	C3'-C2'-C1'	-6.11	95.17	102.50
1	L	112	ARG	CD-NE-CZ	5.89	131.85	123.60
2	C	422	ARG	CG-CD-NE	5.76	123.91	111.80
6	Q	16	DC	O4'-C4'-C3'	-5.62	102.25	104.50
1	K	112	ARG	CD-NE-CZ	5.58	131.42	123.60
7	R	17	DA	O4'-C1'-N9	5.53	111.87	108.00
7	R	13	DT	N3-C4-O4	5.52	123.21	119.90
3	N	311	LEU	CA-CB-CG	5.49	127.92	115.30
7	R	23	DG	O4'-C4'-C3'	-5.42	102.33	104.50
7	H	15	DT	O4'-C1'-N1	5.30	111.71	108.00
7	H	16	DC	C3'-C2'-C1'	-5.25	96.20	102.50
7	H	4	DA	O4'-C1'-N9	-5.20	104.36	108.00
7	H	23	DG	O4'-C1'-N9	5.20	111.64	108.00
7	R	23	DG	C3'-C2'-C1'	-5.14	96.33	102.50
7	R	13	DT	C5-C4-O4	-5.10	121.33	124.90
7	H	6	DT	O4'-C1'-N1	-5.01	104.50	108.00
6	Q	11	DT	N3-C4-O4	5.01	122.90	119.90

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	1782	0	1834	41	0
1	B	1750	0	1797	29	0
1	K	1782	0	1834	35	0
1	L	1773	0	1826	25	0
2	C	8770	0	8874	146	0
2	M	8770	0	8874	158	0
3	D	11738	0	11971	157	0
3	N	11738	0	11971	158	0
4	E	761	0	778	11	0
4	O	761	0	778	12	0
5	F	2807	0	2882	41	0
5	P	2814	0	2889	85	0
6	G	328	0	181	1	0
6	Q	328	0	181	1	0
7	H	495	0	272	12	0
7	R	495	0	272	10	0
8	B	1	0	0	0	0
8	D	3	0	0	0	0
8	F	1	0	0	0	0
8	K	1	0	0	0	0
8	N	3	0	0	0	0
8	P	1	0	0	0	0
9	D	2	0	0	0	0
9	N	2	0	0	0	0
10	A	16	0	0	2	0
10	B	4	0	0	0	0
10	C	104	0	0	8	0
10	D	138	0	0	5	0
10	E	5	0	0	0	0
10	F	32	0	0	3	0
10	G	7	0	0	0	0
10	H	6	0	0	1	0
10	K	12	0	0	0	0
10	L	8	0	0	0	0
10	M	58	0	0	1	0
10	N	89	0	0	2	0
10	O	6	0	0	0	0
10	P	21	0	0	0	0
10	Q	3	0	0	0	0
10	R	5	0	0	0	0
All	All	57420	0	57214	835	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 7.

All (835) 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)
5:P:415:THR:HG22	5:P:416:ARG:CG	1.50	1.41
5:P:415:THR:CG2	5:P:416:ARG:HG3	1.51	1.40
2:M:172:ILE:HG13	2:M:186:VAL:HG22	1.19	1.14
5:P:415:THR:HG22	5:P:416:ARG:CD	1.89	1.01
2:C:627:ARG:NH1	2:C:638:ASP:OD2	1.92	1.01
1:B:112:ARG:NH1	1:B:126:ASP:OD1	1.98	0.96
2:M:1056:LYS:NZ	10:M:1209:HOH:O	1.98	0.95
5:P:415:THR:HG22	5:P:416:ARG:NE	1.81	0.95
5:P:415:THR:CG2	5:P:416:ARG:NE	2.30	0.95
2:M:172:ILE:CG1	2:M:186:VAL:HG22	1.96	0.95
5:P:90:GLN:HA	5:P:90:GLN:NE2	1.85	0.90
2:C:591:SER:O	2:C:592:LEU:HB2	1.70	0.88
3:D:238:PRO:HD3	3:D:318:ARG:HG3	1.56	0.86
5:P:90:GLN:CA	5:P:90:GLN:NE2	2.38	0.86
1:A:112:ARG:HH21	1:A:112:ARG:HG2	1.40	0.86
5:P:90:GLN:N	5:P:90:GLN:HE21	1.75	0.85
5:P:415:THR:HG22	5:P:416:ARG:HG3	0.86	0.85
5:P:410:TYR:O	5:P:414:ARG:HB2	1.77	0.83
5:P:415:THR:HG23	5:P:416:ARG:HG3	1.61	0.83
1:B:111:ALA:HB3	1:B:125:PRO:HA	1.61	0.82
5:P:411:HIS:O	5:P:415:THR:HB	1.79	0.82
2:C:168:ARG:NH2	2:C:265:ARG:O	2.12	0.82
2:M:266:ARG:NH1	7:R:11:DG:N7	2.27	0.81
2:M:628:PHE:H	2:M:638:ASP:HB2	1.45	0.81
5:P:415:THR:CG2	5:P:416:ARG:CG	2.30	0.81
5:P:417:LYS:O	5:P:417:LYS:HG2	1.81	0.79
2:M:591:SER:O	2:M:592:LEU:HB2	1.83	0.78
2:M:905:ILE:HG23	2:M:906:PHE:HD2	1.48	0.78
5:P:414:ARG:N	5:P:414:ARG:HD3	1.99	0.77
3:N:675:ARG:NH2	5:P:420:ASP:OD1	2.17	0.77
5:P:140:ARG:HG3	5:P:142:ARG:HH22	1.50	0.77
2:C:628:PHE:H	2:C:638:ASP:HB2	1.50	0.77
2:C:905:ILE:HG23	2:C:906:PHE:HD2	1.49	0.76
1:L:206:THR:HG22	1:L:209:GLU:H	1.51	0.75
3:D:1254:GLN:HB3	3:D:1258:ARG:HB2	1.69	0.75
3:N:128:TYR:OH	3:N:579:ASP:OD2	2.04	0.75
3:N:1310:ARG:HB2	3:N:1327:ARG:HB2	1.68	0.75
3:N:1254:GLN:HB3	3:N:1258:ARG:HB2	1.68	0.75
5:P:90:GLN:CA	5:P:90:GLN:HE21	1.98	0.75
7:R:13:DT:H5"	7:R:13:DT:H6	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:THR:HG22	1:B:209:GLU:H	1.50	0.74
2:M:462:ASP:HB3	2:M:468:ARG:HD2	1.70	0.73
5:F:397:ILE:HD12	5:F:400:ILE:HD11	1.70	0.73
5:P:412:GLU:HA	5:P:416:ARG:NE	2.04	0.73
3:N:218:LYS:HG2	3:N:338:GLU:HG2	1.70	0.73
2:M:428:ARG:NH2	2:M:447:ALA:O	2.21	0.72
2:C:462:ASP:HB3	2:C:468:ARG:HD2	1.72	0.72
2:M:983:ILE:HG21	2:M:987:ILE:HD11	1.70	0.72
2:C:1056:LYS:NZ	10:C:1208:HOH:O	2.21	0.72
5:P:417:LYS:O	5:P:417:LYS:CG	2.32	0.72
2:C:709:GLU:OE2	2:C:824:ARG:NH1	2.22	0.72
3:D:124:GLU:OE2	3:D:587:ARG:NH2	2.22	0.72
2:C:428:ARG:NH2	2:C:447:ALA:O	2.22	0.72
1:A:112:ARG:CG	1:A:112:ARG:HH21	1.99	0.71
3:D:218:LYS:HG2	3:D:338:GLU:HG2	1.71	0.71
2:M:422:ARG:HH21	7:R:14:DG:H3'	1.53	0.71
2:M:78:PHE:HB3	2:M:82:GLU:HG2	1.71	0.71
5:F:188:ILE:HD13	5:F:221:ILE:HG12	1.73	0.71
2:C:983:ILE:HG21	2:C:987:ILE:HD11	1.72	0.71
3:N:633:VAL:O	3:N:633:VAL:HG13	1.91	0.70
2:M:172:ILE:HG13	2:M:186:VAL:CG2	2.11	0.70
3:D:1208:ASP:C	3:D:1208:ASP:OD1	2.31	0.69
2:M:773:LEU:HD23	5:P:354:LEU:HD13	1.74	0.69
2:M:144:PRO:HG2	2:M:165:LEU:HD23	1.74	0.69
3:N:520:LEU:O	3:N:525:ARG:NH1	2.25	0.69
3:D:142:LEU:HB2	3:D:161:LEU:HD11	1.73	0.69
3:N:1498:ALA:HB1	4:O:84:ARG:HH21	1.58	0.69
2:M:802:ARG:HB2	2:M:826:TYR:HB2	1.75	0.69
5:F:166:LEU:HD13	5:F:170:HIS:HB3	1.75	0.68
3:N:142:LEU:HB2	3:N:161:LEU:HD11	1.74	0.68
3:D:520:LEU:O	3:D:525:ARG:NH1	2.26	0.68
3:N:1282:ARG:NH1	3:N:1295:GLU:OE2	2.27	0.68
3:N:1108:ARG:NH2	3:N:1198:TYR:O	2.26	0.68
2:M:627:ARG:NE	2:M:639:GLN:O	2.27	0.68
3:D:1108:ARG:NH2	3:D:1198:TYR:O	2.26	0.67
3:N:1040:GLY:O	3:N:1060:SER:HB3	1.94	0.67
3:N:1208:ASP:C	3:N:1208:ASP:OD1	2.30	0.67
3:N:124:GLU:OE2	3:N:587:ARG:NH2	2.28	0.67
5:P:273:ARG:HG2	5:P:276:ARG:HH12	1.58	0.67
3:N:36:THR:HG23	3:N:38:LYS:H	1.59	0.67
3:D:260:GLU:OE1	3:D:273:ARG:NH1	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:266:ARG:NH1	7:H:11:DG:N7	2.43	0.66
2:C:210:GLU:HB3	2:C:211:LEU:HD12	1.77	0.66
1:A:112:ARG:NH1	1:A:126:ASP:OD2	2.28	0.66
2:M:172:ILE:CG1	2:M:186:VAL:CG2	2.71	0.66
2:C:683:ASN:HB3	2:C:872:ASN:HD22	1.59	0.65
5:P:361:LEU:HD12	5:P:362:SER:H	1.60	0.65
3:D:128:TYR:OH	3:D:579:ASP:OD2	2.13	0.65
3:D:61:GLY:O	3:D:64:LYS:NZ	2.28	0.65
2:M:1116:ALA:HB2	3:N:88:TYR:HB3	1.78	0.65
1:K:193:ASP:OD2	2:M:938:LYS:NZ	2.19	0.65
2:M:683:ASN:HB3	2:M:872:ASN:HD22	1.61	0.65
3:N:134:VAL:HG12	3:N:454:ALA:HB2	1.79	0.65
2:C:167:LYS:HD3	7:H:12:DC:H5	1.62	0.65
5:P:383:LEU:HD22	5:P:383:LEU:H	1.62	0.65
5:P:91:VAL:O	5:P:193:ARG:NH1	2.29	0.64
3:N:480:GLU:OE2	3:N:488:ARG:NH2	2.31	0.64
2:M:776:SER:OG	5:P:373:LYS:NZ	2.27	0.64
2:C:55:GLU:O	2:C:56:GLU:HB3	1.97	0.64
3:N:1258:ARG:HH21	3:N:1351:GLU:HG2	1.63	0.64
5:P:414:ARG:CD	5:P:414:ARG:N	2.61	0.64
2:M:1059:ASP:OD1	2:M:1059:ASP:C	2.36	0.63
3:D:371:ILE:HG23	5:F:230:LYS:HD2	1.79	0.63
2:C:164:PRO:HD2	2:C:171:TRP:CD1	2.33	0.63
3:D:480:GLU:OE2	3:D:488:ARG:NH2	2.31	0.63
2:C:521:PRO:HB3	3:D:1068:LEU:HD21	1.80	0.63
3:D:1495:ILE:HG12	4:E:88:GLU:HG3	1.80	0.63
1:A:112:ARG:CG	1:A:112:ARG:NH2	2.60	0.62
2:M:236:ILE:HG23	2:M:248:PRO:HB3	1.80	0.62
3:D:621:LYS:NZ	10:D:2143:HOH:O	2.34	0.61
2:M:409:ARG:HG2	2:M:409:ARG:NH1	2.15	0.61
2:C:853:LEU:HB2	2:C:858:MET:HE1	1.83	0.61
1:K:179:PHE:HB3	1:K:197:LEU:HD23	1.83	0.61
2:C:1116:ALA:HB2	3:D:88:TYR:HB3	1.82	0.61
5:P:415:THR:CG2	5:P:416:ARG:HE	2.13	0.60
2:C:711:GLU:HG2	2:C:822:VAL:HG22	1.82	0.60
3:D:266:GLU:HG3	3:D:314:PRO:HB3	1.82	0.60
1:A:216:GLU:OE2	1:A:219:ARG:NH2	2.34	0.60
2:C:135:VAL:HG23	2:C:395:LYS:HG3	1.83	0.60
1:A:179:PHE:HB3	1:A:197:LEU:HD23	1.82	0.60
2:M:709:GLU:OE2	2:M:824:ARG:NH1	2.35	0.60
3:N:1495:ILE:HG13	4:O:88:GLU:HG3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:222:LEU:HD22	1:L:215:VAL:HG12	1.84	0.60
2:M:141:HIS:CE1	2:M:334:ARG:HD2	2.37	0.60
3:D:1491:THR:HG21	4:E:89:MET:HG2	1.83	0.60
1:K:104:GLU:OE2	1:K:137:ARG:NH1	2.35	0.60
2:C:211:LEU:HD11	2:C:304:LEU:HD11	1.82	0.59
3:D:1372:VAL:HA	3:D:1375:MET:HE3	1.84	0.59
2:M:171:TRP:CE3	7:R:13:DT:H2'	2.37	0.59
1:A:24:VAL:HG22	1:A:196:THR:HG23	1.83	0.59
7:R:12:DC:H1'	7:R:13:DT:C5	2.37	0.59
1:K:216:GLU:OE2	1:K:219:ARG:NH2	2.36	0.59
7:H:5:DA:N6	10:H:101:HOH:O	2.35	0.59
2:M:343:GLN:HG3	2:M:385:PHE:HB2	1.83	0.59
1:A:104:GLU:OE2	1:A:137:ARG:NH1	2.35	0.59
5:F:364:ARG:NH1	10:F:2101:HOH:O	2.36	0.59
3:D:45:PHE:O	3:D:86:ARG:NH2	2.36	0.59
5:F:365:GLU:HB2	5:F:404:ALA:HB2	1.83	0.59
5:P:167:PRO:HG2	5:P:170:HIS:HB2	1.85	0.58
2:C:243:ARG:NH2	7:H:9:DG:O6	2.22	0.58
1:A:106:PRO:HG3	1:A:134:GLU:HG2	1.85	0.58
2:C:802:ARG:HB2	2:C:826:TYR:HB2	1.85	0.58
5:P:89:GLY:C	5:P:90:GLN:HE21	2.05	0.58
2:M:409:ARG:HH11	2:M:409:ARG:HG2	1.68	0.58
5:F:361:LEU:HB3	5:F:365:GLU:HG3	1.85	0.58
3:D:1071:PHE:O	3:D:1074:SER:OG	2.22	0.58
2:C:766:GLU:HG3	3:D:64:LYS:HD2	1.85	0.58
1:A:198:ARG:HD3	2:C:934:PHE:CZ	2.37	0.58
5:P:412:GLU:O	5:P:416:ARG:HD2	2.03	0.58
1:A:222:LEU:HD22	1:B:215:VAL:HG12	1.85	0.58
5:P:415:THR:C	5:P:416:ARG:HG3	2.17	0.58
2:C:343:GLN:HG3	2:C:385:PHE:HB2	1.85	0.58
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.86	0.57
2:C:270:GLY:HA3	10:C:1298:HOH:O	2.04	0.57
1:K:24:VAL:HG22	1:K:196:THR:HG23	1.85	0.57
3:N:1143:GLY:O	3:N:1147:ARG:HD2	2.04	0.57
2:C:617:ASP:OD1	2:C:617:ASP:N	2.37	0.57
5:P:360:LYS:NZ	5:P:416:ARG:HH22	2.02	0.57
2:C:422:ARG:HG2	7:H:15:DT:OP2	2.04	0.57
2:M:617:ASP:OD1	2:M:617:ASP:N	2.38	0.57
2:M:683:ASN:HB3	2:M:872:ASN:HB2	1.87	0.56
3:D:1040:GLY:O	3:D:1060:SER:HB3	2.06	0.56
1:K:106:PRO:HG3	1:K:134:GLU:HG2	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:853:LEU:HB2	2:M:858:MET:HE1	1.88	0.56
2:M:177:GLU:HG3	2:M:178:PRO:HD2	1.88	0.56
1:K:64:GLU:HG2	1:K:76:VAL:HG22	1.88	0.56
5:F:393:THR:HG22	5:F:395:GLU:H	1.69	0.56
3:D:134:VAL:HG12	3:D:454:ALA:HB2	1.88	0.56
1:K:184:THR:O	1:K:192:LEU:HB2	2.06	0.56
3:N:828:LYS:HG2	3:N:833:GLU:HB3	1.88	0.56
3:D:828:LYS:HG2	3:D:833:GLU:HB3	1.88	0.56
3:N:1295:GLU:HG2	3:N:1300:SER:HB2	1.88	0.55
5:P:386:VAL:HG22	5:P:397:ILE:HD13	1.88	0.55
2:M:577:PRO:HG2	2:M:580:MET:HG2	1.87	0.55
2:C:853:LEU:HB2	2:C:858:MET:CE	2.36	0.55
3:D:1478:SER:O	3:D:1482:ARG:HB2	2.06	0.55
5:F:193:ARG:HB3	7:H:7:DG:H5"	1.88	0.55
1:K:222:LEU:HD21	1:L:218:LEU:HD23	1.88	0.55
2:C:136:ILE:HB	2:C:336:VAL:HG13	1.87	0.55
1:L:83:LYS:HE2	1:L:168:ASP:HB2	1.88	0.55
3:D:841:TYR:HB2	3:D:864:VAL:HG22	1.89	0.55
5:F:187:LEU:HD23	5:F:224:VAL:HG13	1.89	0.55
3:N:841:TYR:HB2	3:N:864:VAL:HG22	1.89	0.55
2:M:853:LEU:HB2	2:M:858:MET:CE	2.37	0.55
2:M:936:VAL:HG11	2:M:959:PRO:HB2	1.89	0.55
1:A:64:GLU:HG2	1:A:76:VAL:HG22	1.89	0.54
3:N:984:THR:HG22	3:N:987:GLU:H	1.72	0.54
4:O:90:GLU:HG2	4:O:95:VAL:CG2	2.36	0.54
2:C:395:LYS:HD3	2:C:403:SER:HB3	1.89	0.54
3:D:1379:VAL:HG21	3:D:1400:VAL:HG11	1.90	0.54
2:M:68:PHE:HA	2:M:98:LEU:HD23	1.89	0.54
5:P:415:THR:HB	5:P:416:ARG:HE	1.72	0.54
2:M:418:LEU:HD21	2:M:427:VAL:HG11	1.89	0.54
1:L:80:LEU:HG	3:N:844:ALA:HA	1.90	0.54
3:D:434:ARG:NH2	5:F:135:ILE:O	2.40	0.54
2:C:617:ASP:HB2	2:C:619:ARG:HG2	1.89	0.54
2:C:708:TYR:OH	2:C:796:GLU:OE1	2.18	0.54
2:M:905:ILE:HG23	2:M:906:PHE:CD2	2.37	0.54
3:N:1205:TYR:CE1	3:N:1366:LYS:HD2	2.42	0.54
2:C:936:VAL:HG11	2:C:959:PRO:HB2	1.90	0.54
1:L:56:VAL:HG21	1:L:82:LEU:HD13	1.90	0.54
2:M:3:ILE:HD13	2:M:900:ARG:HB2	1.90	0.54
2:C:177:GLU:HG3	2:C:178:PRO:HD2	1.89	0.54
2:C:915:LYS:NZ	3:D:952:ASP:OD2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:ARG:NH1	1:B:126:ASP:CG	2.62	0.54
2:M:607:ASP:HB2	2:M:610:ARG:NH1	2.23	0.54
2:M:212:GLY:HA2	2:M:218:VAL:HG11	1.90	0.54
5:P:418:LEU:HD23	5:P:418:LEU:O	2.08	0.54
2:M:627:ARG:NH1	2:M:638:ASP:OD2	2.41	0.53
2:C:577:PRO:HG2	2:C:580:MET:HG2	1.89	0.53
3:N:239:GLY:O	3:N:312:ARG:NH2	2.40	0.53
1:A:193:ASP:OD1	2:C:938:LYS:NZ	2.35	0.53
1:B:56:VAL:HG21	1:B:82:LEU:HD13	1.90	0.53
2:C:563:ASN:O	2:C:566:THR:HB	2.07	0.53
2:M:628:PHE:H	2:M:638:ASP:CB	2.20	0.53
2:M:617:ASP:HB2	2:M:619:ARG:HG2	1.89	0.53
2:C:607:ASP:HB2	2:C:610:ARG:NH1	2.24	0.53
3:N:1497:GLU:HA	3:N:1500:LYS:HB2	1.90	0.53
2:M:136:ILE:HB	2:M:336:VAL:HG13	1.90	0.53
1:K:220:GLU:O	1:K:223:THR:HB	2.07	0.53
2:M:198:ARG:NE	2:M:229:MET:O	2.31	0.53
2:M:775:ARG:HD3	2:M:782:ALA:HB2	1.90	0.53
2:M:563:ASN:O	2:M:566:THR:HB	2.08	0.53
3:N:1372:VAL:HA	3:N:1375:MET:HE3	1.90	0.53
3:N:90:MET:HG2	3:N:521:PRO:HD3	1.90	0.53
3:D:1150:ALA:HB3	3:D:1187:PRO:HB2	1.90	0.53
3:N:1252:ILE:HG23	3:N:1253:THR:HG23	1.90	0.53
1:B:71:VAL:HG22	1:B:132:LEU:HG	1.91	0.53
2:M:521:PRO:HB3	3:N:1068:LEU:HD21	1.90	0.53
3:D:904:VAL:HG22	3:D:905:PRO:HD2	1.90	0.53
2:M:1006:HIS:HB2	2:M:1024:LYS:HG3	1.90	0.53
3:D:44:LEU:HB3	3:D:525:ARG:NH2	2.24	0.53
2:C:1058:ASP:OD2	3:D:621:LYS:HE2	2.09	0.53
3:N:314:PRO:HB2	3:N:317:VAL:HG12	1.90	0.53
5:F:120:THR:HG21	5:F:122:LEU:HD22	1.91	0.53
3:N:633:VAL:O	3:N:633:VAL:CG1	2.57	0.53
1:B:83:LYS:HE2	1:B:168:ASP:HB2	1.90	0.53
2:M:1106:ASP:OD1	3:N:7:LYS:NZ	2.25	0.53
2:M:217:LEU:HD13	2:M:217:LEU:H	1.74	0.53
2:C:422:ARG:NH2	7:H:14:DG:H3'	2.24	0.52
3:D:1461:GLY:O	3:D:1465:ASN:ND2	2.41	0.52
2:M:12:VAL:HG11	2:M:472:ARG:HD3	1.91	0.52
3:N:643:GLY:HA3	3:N:727:GLN:HB2	1.90	0.52
4:E:45:ARG:NH1	4:E:56:ASP:OD2	2.43	0.52
3:N:1093:TYR:OH	3:N:1441:GLN:OE1	2.19	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:425:PHE:CE2	3:N:1086:LEU:HD12	2.45	0.52
1:L:71:VAL:HG22	1:L:132:LEU:HG	1.92	0.52
1:B:111:ALA:HB3	1:B:125:PRO:CA	2.36	0.52
1:A:57:TYR:CD1	1:A:161:ARG:HD2	2.45	0.52
4:O:45:ARG:NH1	4:O:56:ASP:OD2	2.42	0.52
5:F:153:PRO:HA	5:F:156:VAL:HG22	1.91	0.52
2:C:547:ILE:O	2:C:905:ILE:HD11	2.09	0.52
2:C:418:LEU:HD21	2:C:427:VAL:HG11	1.90	0.52
3:D:242:LEU:HB3	3:D:311:LEU:HD12	1.91	0.52
1:L:80:LEU:HB3	3:N:867:ARG:NH2	2.24	0.52
1:A:94:LEU:O	1:A:146:ARG:NH1	2.43	0.52
3:N:1274:ILE:HG22	3:N:1324:PRO:HA	1.92	0.52
1:A:220:GLU:O	1:A:223:THR:HB	2.09	0.52
3:N:1147:ARG:HD3	3:N:1188:VAL:HG11	1.91	0.52
2:M:704:HIS:CD2	2:M:831:ARG:HD2	2.44	0.52
3:N:1497:GLU:O	3:N:1501:GLU:HG2	2.10	0.52
3:N:411:THR:HB	3:N:437:VAL:H	1.75	0.52
3:D:273:ARG:HB3	3:D:278:PRO:HA	1.92	0.52
3:D:1377:LYS:HE3	3:D:1378:TYR:CZ	2.45	0.52
5:P:415:THR:CB	5:P:416:ARG:HE	2.23	0.52
3:N:904:VAL:HG22	3:N:905:PRO:HD2	1.91	0.52
3:D:1444:THR:O	3:D:1448:THR:HG23	2.09	0.52
2:C:74:GLY:HA3	2:C:93:PRO:HG2	1.92	0.51
3:D:1216:SER:N	10:D:2121:HOH:O	2.43	0.51
1:K:57:TYR:CD1	1:K:161:ARG:HD2	2.45	0.51
2:C:77:PRO:HB2	2:C:78:PHE:CD1	2.45	0.51
3:D:1493:LYS:O	3:D:1497:GLU:HG2	2.10	0.51
3:N:1498:ALA:HB1	4:O:84:ARG:NH2	2.24	0.51
1:B:92:PRO:O	1:B:146:ARG:NH1	2.41	0.51
2:C:405:ARG:HD2	2:C:442:GLU:OE2	2.10	0.51
3:D:411:THR:HB	3:D:437:VAL:H	1.75	0.51
3:D:1046:GLN:N	3:D:1046:GLN:OE1	2.40	0.51
5:P:387:GLY:HA2	5:P:397:ILE:HD12	1.91	0.51
2:C:922:PHE:CE2	2:C:964:LYS:HB2	2.46	0.51
3:D:1272:ALA:HA	3:D:1326:THR:HB	1.92	0.51
2:C:1100:GLN:HG3	10:D:2172:HOH:O	2.11	0.51
2:M:614:ARG:NH2	2:M:618:GLY:O	2.43	0.51
5:P:412:GLU:HA	5:P:416:ARG:CZ	2.40	0.51
1:K:94:LEU:O	1:K:146:ARG:NH1	2.44	0.51
5:P:408:LEU:O	5:P:412:GLU:HB2	2.10	0.51
3:D:192:ALA:HB3	3:D:195:VAL:HB	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:413:LEU:HD21	2:C:451:LEU:HD13	1.92	0.51
5:P:127:ILE:O	5:P:131:VAL:HG23	2.11	0.51
3:N:171:LEU:HD22	3:N:390:PRO:HG2	1.90	0.51
2:M:405:ARG:HD2	2:M:442:GLU:OE2	2.10	0.51
2:M:922:PHE:CE2	2:M:964:LYS:HB2	2.45	0.51
2:C:1006:HIS:HB2	2:C:1024:LYS:HG3	1.91	0.51
1:A:206:THR:HB	1:A:209:GLU:HG3	1.93	0.51
3:N:1189:ARG:HB3	3:N:1204:CYS:HA	1.93	0.51
3:N:192:ALA:HB3	3:N:195:VAL:HB	1.93	0.51
5:F:400:ILE:HG22	5:F:403:LYS:HE2	1.91	0.51
2:M:605:LYS:HB2	2:M:612:VAL:HB	1.93	0.51
2:M:547:ILE:O	2:M:905:ILE:HD11	2.11	0.50
3:D:1258:ARG:HH21	3:D:1351:GLU:HG2	1.75	0.50
3:D:5:VAL:O	3:D:1470:ARG:NH2	2.44	0.50
3:N:897:TRP:CH2	3:N:902:LEU:HD22	2.46	0.50
2:M:708:TYR:HB3	2:M:790:LEU:HD21	1.92	0.50
2:C:679:PHE:HA	3:D:943:THR:HB	1.94	0.50
3:N:1444:THR:O	3:N:1448:THR:HG23	2.12	0.50
3:D:1053:PHE:CZ	3:D:1072:ILE:HD12	2.46	0.50
3:N:131:LYS:O	3:N:456:MET:HG2	2.11	0.50
2:M:191:PHE:HB2	2:M:192:PRO:HD2	1.93	0.50
2:C:704:HIS:CD2	2:C:831:ARG:HD2	2.47	0.50
3:N:658:LEU:HA	3:N:661:MET:HE3	1.94	0.50
3:D:1495:ILE:HD13	4:E:80:VAL:HG21	1.93	0.50
1:B:80:LEU:HG	3:D:844:ALA:HA	1.94	0.50
3:N:996:TRP:CD2	3:N:1056:PRO:HG3	2.46	0.50
1:K:206:THR:HB	1:K:209:GLU:HG3	1.94	0.50
2:M:413:LEU:HD21	2:M:451:LEU:HD13	1.92	0.50
2:C:797:GLY:O	2:C:829:GLN:NE2	2.45	0.50
2:C:614:ARG:NH2	2:C:618:GLY:O	2.44	0.50
2:M:419:THR:H	2:M:422:ARG:HD3	1.76	0.50
3:D:903:ASP:OD1	10:D:2146:HOH:O	2.19	0.50
2:M:627:ARG:NH2	2:M:640:ARG:HG3	2.27	0.50
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.93	0.50
3:N:658:LEU:HD23	3:N:661:MET:HE1	1.94	0.49
2:C:719:PRO:HB3	2:C:820:ARG:NE	2.27	0.49
2:M:758:ARG:HH21	2:M:788:THR:HB	1.76	0.49
5:P:410:TYR:O	5:P:414:ARG:CB	2.55	0.49
2:C:905:ILE:HG23	2:C:906:PHE:CD2	2.38	0.49
1:K:39:PRO:HG3	1:L:39:PRO:HG3	1.94	0.49
1:A:184:THR:O	1:A:192:LEU:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:605:LYS:HB2	2:C:612:VAL:HB	1.94	0.49
5:F:163:LEU:HD13	5:F:174:LEU:HD13	1.95	0.49
2:C:1037:VAL:HG13	2:C:1049:LEU:HD11	1.94	0.49
5:P:414:ARG:HD3	5:P:414:ARG:H	1.75	0.49
3:D:171:LEU:HD22	3:D:390:PRO:HG2	1.94	0.49
3:D:288:MET:HE3	3:D:305:ALA:HB3	1.95	0.49
3:D:860:LEU:O	3:D:876:SER:HB2	2.13	0.49
1:A:188:GLN:O	1:A:188:GLN:OE1	2.30	0.49
2:M:598:GLU:O	2:M:651:LYS:HG3	2.13	0.49
5:P:370:LYS:HB3	5:P:376:ILE:HD13	1.94	0.49
3:D:897:TRP:CH2	3:D:902:LEU:HD22	2.48	0.49
1:A:70:GLY:N	2:C:607:ASP:OD1	2.46	0.49
2:C:787:ASP:OD2	2:C:791:ARG:NH2	2.46	0.49
2:M:189:ARG:NH1	2:M:242:LEU:O	2.46	0.49
2:M:915:LYS:NZ	3:N:952:ASP:OD2	2.46	0.49
2:M:351:LEU:HD12	2:M:375:SER:HA	1.94	0.49
2:M:35:PRO:HG2	2:M:38:LYS:HD3	1.94	0.49
3:N:270:LEU:HD23	3:N:284:LEU:HD11	1.94	0.49
5:P:415:THR:HG21	5:P:416:ARG:NE	2.20	0.48
3:N:1208:ASP:HB2	3:N:1215:VAL:HG23	1.94	0.48
3:N:832:ARG:HD2	3:N:833:GLU:H	1.78	0.48
2:C:872:ASN:ND2	3:D:784:ASP:OD1	2.41	0.48
3:N:1147:ARG:NH2	3:N:1369:GLU:OE1	2.40	0.48
2:C:805:ARG:HG3	2:C:823:VAL:HG22	1.95	0.48
2:C:740:GLU:HB3	2:C:805:ARG:NH1	2.28	0.48
1:L:216:GLU:OE1	1:L:219:ARG:NH2	2.36	0.48
3:D:355:VAL:HG13	3:D:359:ALA:CB	2.43	0.48
3:D:832:ARG:HD2	3:D:833:GLU:H	1.78	0.48
1:A:188:GLN:HB3	1:A:189:ARG:HG2	1.96	0.48
3:D:1068:LEU:O	3:D:1072:ILE:HG12	2.13	0.48
3:D:248:PRO:HG3	3:D:308:LYS:HE3	1.96	0.48
5:F:372:ARG:HG2	5:F:386:VAL:HG21	1.94	0.48
1:B:216:GLU:OE1	1:B:219:ARG:NH2	2.36	0.48
3:N:1042:ARG:HB3	3:N:1057:VAL:HB	1.95	0.48
2:M:682:TYR:CE1	3:N:635:PRO:HD2	2.48	0.48
3:D:1277:ILE:HG22	3:D:1278:ASP:H	1.78	0.48
2:M:211:LEU:HD23	2:M:218:VAL:HG13	1.96	0.48
3:D:236:TYR:CD2	3:D:322:VAL:HG21	2.49	0.48
2:C:17:PRO:HB2	2:C:20:GLU:HB3	1.96	0.48
3:N:1281:VAL:HB	3:N:1317:ASP:H	1.78	0.48
1:L:92:PRO:O	1:L:146:ARG:NH1	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1258:ARG:NH2	3:N:1351:GLU:HG2	2.28	0.48
5:P:354:LEU:O	5:P:358:LEU:HB2	2.14	0.48
3:N:860:LEU:O	3:N:876:SER:HB2	2.13	0.48
2:C:194:VAL:HG22	2:C:221:LEU:HD23	1.95	0.48
3:D:1310:ARG:HD2	3:D:1327:ARG:HD2	1.96	0.48
3:D:808:THR:O	3:D:811:GLU:HB2	2.14	0.48
2:M:577:PRO:HB3	2:M:993:PHE:CG	2.49	0.48
2:C:1043:TYR:CG	3:D:763:MET:HG2	2.49	0.48
3:D:227:LEU:HD13	3:D:331:VAL:HG13	1.96	0.48
3:N:808:THR:O	3:N:811:GLU:HB2	2.14	0.48
1:L:56:VAL:HG22	1:L:142:VAL:HG12	1.96	0.47
3:D:999:THR:O	3:D:1003:VAL:HG13	2.14	0.47
1:B:80:LEU:HD11	3:D:842:VAL:HG12	1.96	0.47
3:D:1100:ASP:OD1	3:D:1463:LYS:NZ	2.35	0.47
1:K:107:LYS:HB2	1:K:107:LYS:HE3	1.73	0.47
2:M:1037:VAL:HG13	2:M:1049:LEU:HD11	1.97	0.47
2:C:683:ASN:HB3	2:C:872:ASN:HB2	1.97	0.47
1:K:27:PRO:HB2	1:K:192:LEU:HD13	1.96	0.47
3:D:959:GLU:HB3	3:D:963:TYR:CE1	2.48	0.47
2:M:64:LEU:N	2:M:103:LYS:HG3	2.28	0.47
5:P:409:LYS:HE2	5:P:409:LYS:HB2	1.76	0.47
2:M:1058:ASP:OD1	3:N:621:LYS:HE2	2.14	0.47
2:M:524:VAL:HG13	2:M:528:GLU:HB2	1.96	0.47
2:C:774:LEU:HD23	5:F:354:LEU:HD21	1.96	0.47
2:M:740:GLU:HB3	2:M:805:ARG:HH12	1.79	0.47
1:L:108:GLU:HG2	1:L:131:THR:HG22	1.96	0.47
2:C:680:ASP:OD1	3:D:943:THR:HG21	2.14	0.47
3:N:260:GLU:OE1	3:N:273:ARG:NH1	2.32	0.47
2:M:397:GLU:N	2:M:633:GLN:OE1	2.41	0.47
2:C:409:ARG:HD2	2:C:452:ILE:HG22	1.95	0.47
3:D:963:TYR:CE2	3:D:1002:LYS:HD3	2.49	0.47
3:D:1219:GLU:HG2	3:D:1221:VAL:HG23	1.95	0.47
3:D:1044:LEU:H	3:D:1044:LEU:HD12	1.78	0.47
2:C:168:ARG:HD3	2:C:268:ASP:CB	2.44	0.47
1:B:56:VAL:HG22	1:B:142:VAL:HG12	1.97	0.47
2:M:911:GLU:O	2:M:915:LYS:HG2	2.15	0.47
3:N:82:LYS:HB2	3:N:84:ILE:HG22	1.95	0.47
3:D:67:ARG:CZ	5:F:379:ARG:HD3	2.45	0.47
3:D:1137:ARG:O	3:D:1141:GLU:HG3	2.14	0.47
2:M:966:LEU:HD13	2:M:986:PRO:HB3	1.96	0.47
2:M:722:ILE:HD12	2:M:821:GLU:HG3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:195:LEU:O	2:M:199:VAL:HG23	2.14	0.47
3:D:1236:LEU:HA	3:D:1359:GLN:HG3	1.96	0.47
1:A:59:GLU:OE1	1:A:139:ASN:ND2	2.44	0.47
1:A:70:GLY:HA3	1:A:136:GLY:HA2	1.97	0.47
5:P:382:THR:OG1	5:P:385:GLU:OE2	2.33	0.47
2:C:1047:HIS:HE1	10:D:2160:HOH:O	1.97	0.47
5:F:270:LYS:HG2	5:F:295:MET:HE1	1.96	0.47
2:C:524:VAL:HG13	2:C:528:GLU:HB2	1.96	0.47
2:M:679:PHE:HA	3:N:943:THR:HB	1.96	0.47
3:D:1263:PHE:HD2	3:D:1375:MET:HE2	1.80	0.47
1:K:70:GLY:N	2:M:607:ASP:OD1	2.47	0.47
3:D:658:LEU:HA	3:D:661:MET:HE3	1.97	0.47
5:F:80:PRO:HB2	5:F:210:LEU:HD11	1.96	0.47
3:N:892:ASP:OD1	3:N:894:LYS:HD2	2.15	0.47
1:B:18:ARG:O	1:B:207:PRO:HD3	2.15	0.47
2:C:436:GLY:HA2	2:C:538:GLN:O	2.15	0.47
5:P:357:ALA:HB1	5:P:408:LEU:HD21	1.97	0.46
5:P:193:ARG:HG2	7:R:7:DG:H5"	1.97	0.46
3:D:658:LEU:HD23	3:D:661:MET:HE1	1.96	0.46
1:L:18:ARG:O	1:L:207:PRO:HD3	2.15	0.46
2:M:194:VAL:HG13	2:M:221:LEU:HG	1.97	0.46
7:H:21:DA:H1'	7:H:22:DT:H5'	1.96	0.46
3:N:984:THR:HG22	3:N:987:GLU:HG3	1.98	0.46
3:N:1068:LEU:O	3:N:1072:ILE:HG12	2.14	0.46
2:C:221:LEU:HD11	2:C:307:LEU:HD21	1.97	0.46
3:D:1312:LEU:HD12	3:D:1324:PRO:HB2	1.97	0.46
2:C:351:LEU:HD12	2:C:375:SER:HA	1.96	0.46
2:M:587:VAL:O	2:M:591:SER:OG	2.30	0.46
3:N:1364:HIS:ND1	3:N:1366:LYS:HB2	2.30	0.46
2:C:911:GLU:O	2:C:915:LYS:HG2	2.16	0.46
3:N:71:LYS:O	3:N:80:VAL:HG22	2.15	0.46
2:M:772:ARG:HE	5:P:373:LYS:HD2	1.80	0.46
2:M:504:GLU:HG2	2:M:509:ALA:HB2	1.98	0.46
3:N:438:ASP:OD1	3:N:441:ARG:NH2	2.49	0.46
2:C:598:GLU:O	2:C:651:LYS:HG3	2.15	0.46
1:A:227:ASN:HA	1:A:228:PRO:HD3	1.75	0.46
1:B:108:GLU:HG2	1:B:131:THR:HG22	1.97	0.46
3:N:1371:VAL:HG12	3:N:1375:MET:HE2	1.97	0.46
2:C:134:ARG:NH1	2:C:392:SER:O	2.49	0.46
3:N:1047:LYS:HG2	3:N:1053:PHE:CZ	2.50	0.46
2:M:797:GLY:O	2:M:829:GLN:NE2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:872:ASN:ND2	3:N:784:ASP:OD1	2.39	0.46
2:C:1057:SER:HB3	2:C:1058:ASP:H	1.51	0.46
3:N:954:ALA:HB3	3:N:1062:ARG:HG3	1.97	0.46
2:M:711:GLU:HG2	2:M:822:VAL:HG22	1.97	0.46
3:D:892:ASP:OD1	3:D:894:LYS:HD2	2.15	0.46
2:C:163:ILE:HG23	2:C:171:TRP:CE2	2.51	0.46
2:C:64:LEU:HD22	2:C:100:LEU:HD11	1.97	0.46
2:C:722:ILE:HD12	2:C:821:GLU:HG3	1.97	0.46
2:C:881:ASN:N	2:C:881:ASN:OD1	2.49	0.46
5:F:201:LYS:NZ	5:F:244:ARG:HH22	2.14	0.46
3:N:44:LEU:HB3	3:N:525:ARG:NH2	2.30	0.46
2:C:580:MET:HB3	2:C:584:GLU:CD	2.36	0.46
3:D:236:TYR:CZ	3:D:242:LEU:HD12	2.51	0.46
1:B:80:LEU:HB3	3:D:867:ARG:NH2	2.31	0.46
5:F:164:LYS:HA	5:F:171:LYS:HE3	1.98	0.46
1:L:49:PRO:HA	1:L:148:VAL:HG12	1.97	0.46
2:C:504:GLU:HG2	2:C:509:ALA:HB2	1.98	0.46
1:A:39:PRO:HG3	1:B:39:PRO:HG3	1.98	0.46
2:C:118:ILE:HD11	2:C:344:PHE:CE2	2.51	0.46
2:C:186:VAL:HG11	2:C:260:LEU:HD21	1.98	0.46
3:N:586:ARG:HH22	6:Q:10:DG:H5"	1.80	0.46
5:F:162:LYS:HE3	5:F:162:LYS:HB2	1.72	0.46
1:K:188:GLN:HG3	1:K:189:ARG:HG3	1.98	0.46
3:D:34:TYR:CZ	3:D:35:ARG:HG3	2.51	0.46
5:P:77:THR:O	5:P:78:SER:CB	2.64	0.45
2:M:69:LEU:HD12	2:M:97:ARG:HG2	1.98	0.45
1:L:124:ASN:OD1	1:L:124:ASN:N	2.49	0.45
3:N:741:ASP:OD1	3:N:743:ASP:OD1	2.34	0.45
7:R:21:DA:C8	7:R:21:DA:H5'	2.51	0.45
7:R:21:DA:H8	7:R:21:DA:H5'	1.82	0.45
4:E:68:LEU:HD12	4:E:68:LEU:HA	1.77	0.45
3:D:1189:ARG:HB3	3:D:1204:CYS:HA	1.98	0.45
7:H:15:DT:H2"	7:H:16:DC:H5'	1.96	0.45
1:K:70:GLY:HA3	1:K:136:GLY:HA2	1.98	0.45
1:A:57:TYR:CG	1:A:161:ARG:HD2	2.52	0.45
2:C:331:ARG:NH2	10:C:1304:HOH:O	2.49	0.45
2:M:216:GLU:H	2:M:216:GLU:CD	2.18	0.45
2:M:397:GLU:HG3	2:M:631:SER:HB2	1.98	0.45
2:C:172:ILE:CG1	2:C:186:VAL:HG22	2.47	0.45
1:L:176:ARG:NH2	3:N:888:GLU:OE1	2.49	0.45
5:F:333:ILE:HA	5:F:334:PRO:HD3	1.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:436:GLY:HA2	2:M:538:GLN:O	2.15	0.45
2:M:328:LEU:HD23	2:M:328:LEU:HA	1.82	0.45
5:P:380:GLU:CD	5:P:380:GLU:H	2.20	0.45
2:C:157:ARG:HA	2:C:157:ARG:HD3	1.77	0.45
3:D:957:PRO:HG3	3:D:1007:VAL:HA	1.99	0.45
2:C:966:LEU:HD13	2:C:986:PRO:HB3	1.97	0.45
1:K:57:TYR:CG	1:K:161:ARG:HD2	2.51	0.45
3:N:1141:GLU:OE1	3:N:1168:MET:HE2	2.16	0.45
1:L:34:VAL:HG12	1:L:181:VAL:HG21	1.99	0.45
4:O:40:LEU:HG	4:O:67:GLU:HG2	1.98	0.45
5:P:415:THR:HG21	5:P:416:ARG:CZ	2.46	0.45
2:M:1102:LEU:HB2	3:N:7:LYS:HB2	1.99	0.45
1:A:186:LEU:C	1:A:188:GLN:H	2.18	0.45
2:M:251:ASP:OD1	2:M:251:ASP:N	2.47	0.45
2:M:187:ASN:HA	2:M:187:ASN:HD22	1.60	0.45
2:C:168:ARG:HD3	2:C:268:ASP:HB3	1.99	0.45
1:L:64:GLU:HA	1:L:165:ILE:HD13	1.99	0.45
2:M:154:ARG:HA	2:M:155:PRO:HD3	1.66	0.45
3:D:230:TRP:CZ2	3:D:232:GLU:HG2	2.51	0.45
2:M:948:GLU:HB3	2:M:953:VAL:HG23	1.98	0.45
1:A:112:ARG:HD2	10:A:412:HOH:O	2.17	0.45
5:F:400:ILE:HA	5:F:403:LYS:HG2	1.98	0.45
3:N:1495:ILE:HD13	4:O:80:VAL:HG21	1.98	0.45
2:M:67:ASP:OD1	2:M:68:PHE:N	2.50	0.45
2:C:247:PRO:HA	2:C:248:PRO:HD3	1.65	0.45
2:M:172:ILE:HG12	2:M:186:VAL:CG2	2.46	0.44
2:C:740:GLU:HB3	2:C:805:ARG:HH12	1.81	0.44
3:N:489:ARG:NH1	3:N:1391:GLU:OE2	2.50	0.44
5:P:364:ARG:HH12	5:P:392:VAL:HG11	1.82	0.44
1:B:34:VAL:HG12	1:B:181:VAL:HG21	1.99	0.44
3:N:1461:GLY:O	3:N:1465:ASN:ND2	2.49	0.44
3:D:131:LYS:O	3:D:456:MET:HG2	2.16	0.44
3:N:59:ALA:HB2	3:N:78:VAL:HG21	1.99	0.44
3:D:134:VAL:HG22	3:D:151:GLN:H	1.82	0.44
3:N:266:GLU:HB3	3:N:314:PRO:HB3	2.00	0.44
3:N:273:ARG:HG2	3:N:278:PRO:HA	1.99	0.44
3:N:1003:VAL:HG21	3:N:1041:LEU:HG	1.98	0.44
1:B:91:ASN:HB3	1:B:94:LEU:HB2	1.99	0.44
2:C:874:LEU:HD23	3:D:1023:MET:SD	2.57	0.44
5:P:329:TYR:CE2	5:P:333:ILE:HD11	2.53	0.44
2:C:12:VAL:HG21	2:C:472:ARG:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:ASN:N	1:B:124:ASN:OD1	2.51	0.44
2:C:6:PHE:CD2	2:C:909:ALA:HB2	2.52	0.44
1:K:115:LEU:HA	1:K:116:PRO:HD3	1.82	0.44
1:B:64:GLU:HA	1:B:165:ILE:HD13	2.00	0.44
2:M:404:LEU:O	2:M:408:ARG:HG3	2.16	0.44
7:H:3:DT:H2'	7:H:4:DA:C8	2.52	0.44
3:D:959:GLU:N	3:D:959:GLU:OE1	2.50	0.44
2:C:76:PRO:HG3	2:C:120:LEU:CD1	2.47	0.44
2:C:408:ARG:NH2	10:C:1210:HOH:O	2.51	0.44
3:N:801:GLY:O	3:N:804:LEU:HG	2.18	0.44
2:C:1001:VAL:HG13	3:D:630:VAL:HB	1.99	0.44
2:M:1054:THR:O	2:M:1059:ASP:HB3	2.18	0.44
3:D:939:PHE:O	3:D:943:THR:HG22	2.18	0.44
2:C:203:ASP:OD2	2:C:204:GLN:N	2.51	0.44
1:K:59:GLU:OE1	1:K:139:ASN:ND2	2.44	0.44
2:C:976:ASP:OD1	2:C:978:ARG:HD3	2.17	0.44
3:N:1232:PRO:HG2	3:N:1356:TYR:HE2	1.82	0.44
2:C:434:HIS:HE1	10:C:1206:HOH:O	2.00	0.44
3:D:801:GLY:O	3:D:804:LEU:HG	2.18	0.44
2:M:858:MET:HG2	2:M:867:VAL:O	2.18	0.44
1:A:206:THR:HG22	1:A:208:LEU:H	1.83	0.44
3:N:689:ASP:O	3:N:693:GLU:HG3	2.18	0.44
5:P:403:LYS:HA	5:P:406:ARG:HG2	1.98	0.44
5:P:188:ILE:HD13	5:P:221:ILE:HG12	1.98	0.44
3:N:134:VAL:HG22	3:N:151:GLN:H	1.82	0.44
3:D:134:VAL:HG23	3:D:149:LYS:HA	2.00	0.44
2:M:395:LYS:HE2	2:M:403:SER:HB3	2.00	0.44
3:D:521:PRO:HA	3:D:522:PRO:HD3	1.90	0.44
3:D:711:LEU:HD13	3:D:778:LEU:HD13	2.00	0.44
2:C:328:LEU:HA	2:C:328:LEU:HD23	1.81	0.44
3:N:939:PHE:O	3:N:943:THR:HG22	2.18	0.44
5:F:370:LYS:HB3	5:F:376:ILE:HG13	2.00	0.44
1:A:8:ALA:HA	1:A:9:PRO:HD3	1.66	0.44
3:D:438:ASP:OD1	3:D:441:ARG:NH2	2.49	0.44
2:C:577:PRO:HB3	2:C:993:PHE:CG	2.53	0.43
5:P:77:THR:HG23	5:P:77:THR:O	2.18	0.43
2:M:28:ARG:HH12	2:M:42:VAL:HG11	1.83	0.43
3:N:536:ALA:HA	5:P:315:VAL:O	2.18	0.43
1:L:80:LEU:HD11	3:N:842:VAL:HG12	2.00	0.43
4:E:45:ARG:HA	4:E:46:PRO:HD3	1.92	0.43
2:C:172:ILE:HG13	2:C:186:VAL:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1042:ARG:HB3	3:D:1057:VAL:HB	2.00	0.43
5:F:392:VAL:HB	5:F:396:ARG:HG2	1.99	0.43
2:M:930:LYS:HE3	2:M:935:GLY:HA2	2.01	0.43
2:M:764:GLU:HG2	3:N:54:LYS:NZ	2.33	0.43
3:N:44:LEU:HB3	3:N:525:ARG:HH21	1.83	0.43
3:N:134:VAL:HG23	3:N:149:LYS:HA	2.01	0.43
3:N:657:LEU:HG	3:N:661:MET:HE2	1.99	0.43
2:M:150:PRO:HG3	2:M:322:VAL:HG11	2.00	0.43
5:F:319:THR:HA	5:F:320:PRO:HD3	1.86	0.43
3:N:46:ASP:HB3	3:N:49:ILE:HD12	2.01	0.43
1:B:49:PRO:HA	1:B:148:VAL:HG12	1.99	0.43
3:N:1018:ASN:HA	3:N:1019:PRO:HD3	1.92	0.43
2:C:404:LEU:O	2:C:408:ARG:HG3	2.18	0.43
1:A:9:PRO:HG3	10:A:407:HOH:O	2.18	0.43
2:C:930:LYS:HE3	2:C:935:GLY:HA2	2.01	0.43
3:D:483:HIS:HA	3:D:484:PRO:HD3	1.91	0.43
2:C:230:ARG:HG3	2:C:233:GLU:HG3	2.00	0.43
2:M:876:VAL:HB	3:N:949:ILE:HD12	2.00	0.43
5:P:412:GLU:HA	5:P:416:ARG:HE	1.81	0.43
2:M:409:ARG:HH11	2:M:409:ARG:CG	2.31	0.43
1:K:6:LEU:HD11	1:K:27:PRO:HG2	1.99	0.43
2:M:1053:LEU:HA	3:N:621:LYS:HD2	2.01	0.43
5:P:333:ILE:HA	5:P:334:PRO:HD3	1.87	0.43
2:C:954:THR:HA	2:C:955:PRO:HD3	1.88	0.43
3:N:1459:LEU:HD12	3:N:1464:GLU:HB3	1.99	0.43
3:D:465:LEU:HD12	3:D:513:ILE:HD13	1.99	0.43
3:D:619:LEU:HD11	3:D:1439:SER:HB2	2.01	0.43
2:M:874:LEU:HD23	3:N:1023:MET:SD	2.58	0.43
3:D:1031:ASN:O	3:D:1035:ILE:HG12	2.19	0.43
3:N:711:LEU:HD13	3:N:778:LEU:HD13	2.00	0.43
3:N:371:ILE:HD12	5:P:230:LYS:HA	2.01	0.43
1:A:107:LYS:HE3	1:A:107:LYS:HB2	1.71	0.43
5:P:371:LEU:HD22	5:P:381:HIS:CE1	2.53	0.43
2:M:1051:GLU:HB3	2:M:1056:LYS:HD2	2.00	0.43
3:D:44:LEU:HB3	3:D:525:ARG:HH21	1.83	0.43
5:P:397:ILE:HA	5:P:400:ILE:HG22	2.01	0.43
2:C:97:ARG:NH1	2:C:110:GLU:OE1	2.51	0.43
2:M:728:HIS:CD2	5:P:422:LEU:HD13	2.53	0.43
1:K:36:LEU:HD23	1:K:36:LEU:HA	1.80	0.43
3:D:1147:ARG:HD3	3:D:1188:VAL:HG11	2.01	0.43
2:C:948:GLU:HB3	2:C:953:VAL:HG23	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:155:THR:O	5:P:159:ILE:HG12	2.19	0.43
2:M:87:ASP:HA	2:M:131:GLY:HA3	2.01	0.43
2:M:202:TYR:CE1	2:M:304:LEU:HD22	2.54	0.43
3:D:17:LYS:HE3	3:D:17:LYS:HB2	1.70	0.43
5:P:410:TYR:O	5:P:414:ARG:HG2	2.18	0.43
2:M:627:ARG:HD2	2:M:627:ARG:HA	1.53	0.43
2:M:211:LEU:HD21	2:M:311:PHE:CE2	2.54	0.43
2:M:1102:LEU:HD23	2:M:1108:PRO:HA	2.01	0.43
2:M:154:ARG:NH2	2:M:157:ARG:HG3	2.33	0.43
3:D:1018:ASN:HA	3:D:1019:PRO:HD3	1.90	0.43
3:D:1126:ASP:OD1	3:D:1128:VAL:HG13	2.18	0.43
3:N:1107:VAL:HA	3:N:1200:VAL:O	2.19	0.43
3:D:1258:ARG:HH21	3:D:1351:GLU:CG	2.32	0.43
1:B:211:LEU:O	1:B:215:VAL:HG22	2.19	0.43
2:C:774:LEU:HA	2:C:774:LEU:HD22	1.82	0.43
3:D:661:MET:HE2	3:D:677:LEU:HD11	2.00	0.43
3:N:589:ALA:HA	3:N:590:PRO:HD3	1.91	0.43
3:D:536:ALA:HA	5:F:315:VAL:O	2.19	0.43
2:C:771:GLU:O	2:C:775:ARG:HB2	2.19	0.43
1:B:44:LEU:HD13	1:B:199:ILE:HD13	2.00	0.43
3:N:1478:SER:O	3:N:1482:ARG:HB2	2.19	0.43
3:N:483:HIS:HA	3:N:484:PRO:HD3	1.91	0.43
3:N:1258:ARG:HH21	3:N:1351:GLU:CG	2.31	0.42
2:M:35:PRO:HA	2:M:36:PRO:HD3	1.95	0.42
2:M:535:SER:O	2:M:538:GLN:HG2	2.18	0.42
2:C:1102:LEU:HD23	2:C:1108:PRO:HA	2.01	0.42
2:M:684:PHE:HE1	3:N:783:ARG:HB2	1.84	0.42
1:A:6:LEU:HD13	1:A:7:LYS:H	1.84	0.42
5:F:338:LEU:HD23	5:F:339:PRO:HD2	2.01	0.42
3:N:879:ARG:HD3	3:N:902:LEU:O	2.19	0.42
2:C:12:VAL:HG11	2:C:472:ARG:HD3	2.01	0.42
2:C:578:VAL:HG22	10:C:1225:HOH:O	2.19	0.42
3:D:689:ASP:O	3:D:693:GLU:HG3	2.19	0.42
3:N:434:ARG:NH2	5:P:135:ILE:O	2.52	0.42
3:N:96:ALA:HB3	3:N:554:LEU:HD23	2.00	0.42
5:F:188:ILE:HG12	5:F:224:VAL:HG21	2.01	0.42
5:P:329:TYR:HE2	5:P:333:ILE:HD11	1.84	0.42
1:K:8:ALA:HA	1:K:9:PRO:HD3	1.65	0.42
3:N:350:HIS:CD2	5:P:232:ARG:HG2	2.53	0.42
3:D:684:LYS:HE2	3:D:684:LYS:HB3	1.85	0.42
3:D:1258:ARG:NH2	3:D:1351:GLU:HG2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:766:GLU:CG	3:D:64:LYS:HD2	2.48	0.42
3:D:1047:LYS:HG2	3:D:1053:PHE:CZ	2.54	0.42
5:F:372:ARG:HD3	5:F:401:GLU:OE2	2.20	0.42
7:R:18:DC:H2"	7:R:19:DG:C8	2.54	0.42
2:C:144:PRO:HG2	2:C:165:LEU:HD23	2.01	0.42
4:O:17:TYR:O	4:O:21:VAL:HG23	2.20	0.42
2:M:348:LEU:HD12	2:M:348:LEU:HA	1.92	0.42
2:M:77:PRO:HB2	2:M:78:PHE:CD1	2.53	0.42
3:N:897:TRP:HH2	3:N:902:LEU:HD22	1.84	0.42
2:M:35:PRO:HG2	2:M:38:LYS:HB2	2.02	0.42
2:M:976:ASP:OD1	2:M:978:ARG:HD3	2.18	0.42
3:D:42:ASP:OD1	3:D:48:ARG:NH2	2.53	0.42
10:C:1268:HOH:O	5:F:280:GLN:HG2	2.18	0.42
1:A:36:LEU:HD23	1:A:36:LEU:HA	1.79	0.42
5:P:89:GLY:C	5:P:90:GLN:NE2	2.70	0.42
1:K:206:THR:HG22	1:K:208:LEU:H	1.84	0.42
1:A:180:GLN:NE2	2:C:935:GLY:O	2.52	0.42
2:M:239:PHE:CD2	2:M:253:ALA:HA	2.53	0.42
2:C:792:VAL:HA	2:C:793:PRO:HD3	1.89	0.42
3:N:1373:ARG:HD3	10:N:2143:HOH:O	2.19	0.42
2:M:230:ARG:HB2	2:M:231:PRO:HD2	2.01	0.42
1:K:201:THR:HG21	1:K:205:VAL:O	2.20	0.42
3:N:47:GLU:CD	3:N:53:ILE:HG12	2.40	0.42
3:N:1304:LYS:HE2	3:N:1304:LYS:HB3	1.86	0.42
5:P:360:LYS:HZ1	5:P:416:ARG:HH22	1.67	0.42
3:D:1144:LEU:HA	3:D:1144:LEU:HD23	1.79	0.42
2:M:592:LEU:HA	2:M:592:LEU:HD23	1.80	0.42
3:D:1053:PHE:CE1	3:D:1072:ILE:HG23	2.55	0.42
3:D:1324:PRO:HG3	3:D:1330:ILE:HD11	2.00	0.42
2:C:229:MET:HB2	2:C:233:GLU:HB2	2.01	0.42
2:C:179:ASN:OD1	2:C:181:VAL:HG12	2.20	0.42
2:C:944:LEU:HD23	2:C:944:LEU:HA	1.92	0.42
3:N:1342:GLU:CD	3:N:1342:GLU:H	2.23	0.42
1:L:156:HIS:ND1	1:L:158:ILE:HG12	2.34	0.42
1:L:211:LEU:O	1:L:215:VAL:HG22	2.20	0.42
3:N:876:SER:OG	3:N:879:ARG:HG3	2.20	0.42
5:P:376:ILE:HG22	5:P:377:ASP:N	2.35	0.42
5:P:384:GLU:HB3	5:P:394:ARG:HD3	2.02	0.42
3:N:1353:GLN:HG2	3:N:1368:ILE:HD12	2.01	0.42
3:N:1284:GLU:HB3	3:N:1291:SER:HB3	2.01	0.42
2:C:269:LEU:HB2	2:C:288:ARG:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:88:ILE:HA	5:F:88:ILE:HD12	1.75	0.42
2:C:858:MET:HG2	2:C:867:VAL:O	2.20	0.41
1:K:6:LEU:HD13	1:K:7:LYS:H	1.85	0.41
2:C:1102:LEU:HB2	3:D:7:LYS:HB2	2.02	0.41
1:A:11:PHE:O	1:B:228:PRO:HA	2.20	0.41
3:N:707:THR:HG23	3:N:712:GLY:HA3	2.01	0.41
3:N:1071:PHE:O	3:N:1074:SER:OG	2.29	0.41
4:E:40:LEU:HG	4:E:67:GLU:HG2	2.01	0.41
3:N:842:VAL:HG22	3:N:865:THR:HB	2.02	0.41
3:D:355:VAL:HG13	3:D:359:ALA:HB3	2.01	0.41
7:R:15:DT:H2"	7:R:16:DC:H5'	2.02	0.41
4:E:3:GLU:HA	4:E:4:PRO:HD3	1.93	0.41
1:B:156:HIS:ND1	1:B:158:ILE:HG12	2.35	0.41
5:P:83:GLN:O	5:P:87:GLU:HG3	2.20	0.41
2:M:657:ASP:OD2	2:M:663:ASN:N	2.48	0.41
3:D:1348:LEU:HA	3:D:1348:LEU:HD23	1.92	0.41
3:D:275:GLU:HB3	3:D:276:ASP:H	1.69	0.41
5:F:193:ARG:HB3	7:H:7:DG:C5'	2.50	0.41
2:M:605:LYS:HB3	2:M:610:ARG:NH1	2.35	0.41
5:F:270:LYS:HE2	5:F:295:MET:HE2	2.01	0.41
2:C:535:SER:O	2:C:538:GLN:HG2	2.20	0.41
5:P:319:THR:HA	5:P:320:PRO:HD3	1.92	0.41
5:F:397:ILE:HA	5:F:400:ILE:HG12	2.02	0.41
3:N:521:PRO:HA	3:N:522:PRO:HD3	1.91	0.41
5:F:273:ARG:NH1	10:F:2108:HOH:O	2.54	0.41
2:C:89:THR:O	2:C:91:GLN:HG2	2.20	0.41
1:L:175:ARG:N	1:L:200:TRP:O	2.50	0.41
3:D:15:PRO:O	3:D:19:ARG:HG3	2.21	0.41
3:D:206:ARG:HD2	3:D:206:ARG:HA	1.76	0.41
2:M:591:SER:O	2:M:592:LEU:CB	2.55	0.41
2:M:580:MET:HB3	2:M:584:GLU:CD	2.41	0.41
3:D:842:VAL:HG22	3:D:865:THR:HB	2.02	0.41
5:P:80:PRO:HB2	5:P:210:LEU:HD11	2.02	0.41
3:N:493:ARG:NH1	10:N:2150:HOH:O	2.48	0.41
2:M:786:LYS:HB3	2:M:786:LYS:HE2	1.81	0.41
4:E:36:LYS:HB3	4:E:36:LYS:HE3	1.81	0.41
1:A:91:ASN:HA	1:A:92:PRO:HD3	1.93	0.41
2:C:1081:VAL:HA	2:C:1082:PRO:HD3	1.93	0.41
3:N:486:ARG:HG3	3:N:486:ARG:H	1.52	0.41
4:O:83:ASP:N	4:O:83:ASP:OD1	2.53	0.41
4:O:14:ASP:N	4:O:14:ASP:OD2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:399:GLN:HG3	5:P:403:LYS:HE2	2.02	0.41
3:D:237:LYS:N	3:D:240:GLU:OE1	2.46	0.41
2:M:942:GLU:HG2	2:M:945:ARG:HH21	1.85	0.41
1:K:11:PHE:O	1:L:228:PRO:HA	2.21	0.41
1:A:201:THR:HG21	1:A:205:VAL:O	2.20	0.41
3:N:206:ARG:HA	3:N:206:ARG:HD2	1.77	0.41
2:C:462:ASP:OD2	2:C:468:ARG:NH1	2.51	0.41
3:N:103:TRP:HB3	3:N:1448:THR:CG2	2.51	0.41
5:P:422:LEU:HD23	5:P:422:LEU:HA	1.89	0.41
3:D:41:ARG:HG3	3:D:48:ARG:HE	1.85	0.41
1:K:41:ARG:HA	1:K:177:VAL:HG11	2.03	0.41
3:N:465:LEU:HD12	3:N:513:ILE:HD13	2.01	0.41
3:D:586:ARG:HH22	6:G:10:DG:H5"	1.86	0.41
10:F:2110:HOH:O	7:H:1:DT:H72	2.21	0.41
5:F:140:ARG:HE	5:F:140:ARG:HB2	1.60	0.41
4:E:14:ASP:N	4:E:14:ASP:OD2	2.54	0.41
1:K:31:GLY:N	1:K:193:ASP:OD1	2.47	0.41
2:C:272:ALA:HB3	10:C:1298:HOH:O	2.20	0.41
2:C:605:LYS:HB3	2:C:610:ARG:NH1	2.36	0.41
2:M:136:ILE:HD13	2:M:392:SER:HA	2.03	0.41
3:N:50:PHE:CD2	3:N:522:PRO:HD3	2.56	0.41
2:M:12:VAL:HG21	2:M:472:ARG:HD3	2.03	0.41
3:D:879:ARG:HD3	3:D:902:LEU:O	2.21	0.41
2:C:1043:TYR:CD1	3:D:763:MET:HG2	2.55	0.41
3:N:84:ILE:O	3:N:87:ARG:HG3	2.21	0.41
2:C:200:LEU:HD13	2:C:300:ASP:HB2	2.02	0.41
2:C:1038:TRP:CE2	3:D:1099:VAL:HG11	2.56	0.41
2:C:160:ALA:HB3	2:C:174:LEU:HB2	2.02	0.41
2:C:939:ARG:H	2:C:939:ARG:HG2	1.67	0.41
1:B:115:LEU:HA	1:B:116:PRO:HD3	1.91	0.41
3:D:618:LEU:HG	3:D:1467:ILE:HG23	2.03	0.41
3:D:1000:THR:HG23	3:D:1036:ARG:HD2	2.03	0.41
1:K:100:LEU:HD23	1:K:141:GLU:HG2	2.03	0.41
2:M:464:LEU:HD12	2:M:464:LEU:HA	1.84	0.41
2:M:944:LEU:HA	2:M:944:LEU:HD23	1.91	0.41
4:O:57:ASP:HA	4:O:58:PRO:HD3	1.89	0.41
3:D:1463:LYS:HB3	3:D:1463:LYS:HE2	1.90	0.41
5:F:79:ASP:HA	5:F:80:PRO:HD3	1.91	0.41
2:M:232:GLU:HG2	2:M:250:ARG:HD2	2.02	0.41
2:C:107:LEU:HD22	2:C:108:ILE:N	2.36	0.41
3:D:1387:SER:HB3	3:D:1407:LEU:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1217:ILE:HD12	3:D:1480:PHE:CZ	2.56	0.41
2:M:1043:TYR:CG	3:N:763:MET:HG2	2.56	0.41
3:N:729:HIS:HA	3:N:730:PRO:HD3	1.96	0.41
3:N:1099:VAL:O	3:N:1103:HIS:HB3	2.21	0.41
3:D:428:LYS:HB3	3:D:428:LYS:HE2	1.93	0.41
4:O:46:PRO:HD2	4:O:63:TRP:CE2	2.56	0.41
2:M:91:GLN:HB2	2:M:117:HIS:HB3	2.02	0.41
3:D:1208:ASP:O	3:D:1208:ASP:OD1	2.39	0.40
3:D:876:SER:OG	3:D:879:ARG:HG3	2.22	0.40
3:D:1003:VAL:O	3:D:1007:VAL:HG23	2.20	0.40
3:D:1122:LEU:HD13	3:D:1178:ALA:HB2	2.03	0.40
2:C:236:ILE:O	2:C:240:THR:HG23	2.20	0.40
2:M:561:GLY:O	2:M:565:GLN:HG3	2.21	0.40
1:L:91:ASN:HB3	1:L:94:LEU:HB2	2.02	0.40
2:C:642:ARG:HA	2:C:642:ARG:HD3	1.84	0.40
3:N:684:LYS:HE2	3:N:684:LYS:HB3	1.85	0.40
3:D:314:PRO:HB2	3:D:317:VAL:HG12	2.03	0.40
3:D:657:LEU:HG	3:D:661:MET:HE2	2.03	0.40
2:M:232:GLU:CG	2:M:250:ARG:HD2	2.51	0.40
2:C:942:GLU:HG2	2:C:945:ARG:HH21	1.85	0.40
2:M:593:ALA:HB1	2:M:659:PRO:HD2	2.03	0.40
3:D:405:ASP:CG	3:D:406:ASP:H	2.25	0.40
3:N:1383:ASP:HA	3:N:1384:PRO:HD3	1.84	0.40
3:N:1010:ASN:OD1	3:N:1014:ASN:ND2	2.47	0.40
3:D:1205:TYR:CZ	3:D:1366:LYS:HD3	2.56	0.40
3:N:731:LEU:HA	3:N:731:LEU:HD23	1.92	0.40
3:N:468:LEU:HA	3:N:468:LEU:HD23	1.92	0.40
3:N:219:GLU:HB2	3:N:339:TRP:HH2	1.86	0.40
5:P:140:ARG:CG	5:P:142:ARG:HH22	2.27	0.40
1:A:188:GLN:C	1:A:188:GLN:OE1	2.60	0.40
3:D:462:GLN:HB2	3:D:513:ILE:HG21	2.02	0.40
3:D:114:THR:HG23	3:D:495:ARG:HG2	2.03	0.40
5:P:256:ARG:NH2	5:P:311:ALA:O	2.54	0.40
2:M:881:ASN:OD1	2:M:881:ASN:N	2.50	0.40
5:F:364:ARG:HG2	5:F:390:PHE:CE2	2.57	0.40
2:M:135:VAL:HG23	2:M:395:LYS:HG3	2.03	0.40
1:K:32:PHE:HA	1:K:35:THR:HB	2.03	0.40
3:D:834:THR:OG1	3:D:838:ARG:HD2	2.22	0.40
3:D:1487:VAL:HG11	3:D:1492:LEU:HD23	2.03	0.40
5:P:84:TYR:CZ	5:P:88:ILE:HD11	2.56	0.40
5:P:88:ILE:HD13	5:P:88:ILE:HA	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:365:GLU:HA	5:P:368:VAL:HG22	2.03	0.40
3:N:834:THR:OG1	3:N:838:ARG:HD2	2.21	0.40
1:K:65:PHE:O	2:M:628:PHE:CE2	2.75	0.40
3:N:952:ASP:HA	3:N:1062:ARG:NH2	2.36	0.40
3:N:284:LEU:HA	3:N:285:PRO:HD2	1.94	0.40
2:M:1057:SER:HB3	2:M:1058:ASP:H	1.55	0.40
3:N:487:ALA:O	3:N:491:LYS:HG2	2.21	0.40
3:D:890:VAL:HB	3:D:922:LEU:HD13	2.04	0.40
3:D:475:LYS:O	3:D:479:GLU:HG2	2.22	0.40
2:M:571:LEU:HD22	2:M:700:TYR:HA	2.02	0.40
1:A:111:ALA:HB3	1:A:125:PRO:HA	2.04	0.40
3:N:1468:LEU:HB3	3:N:1470:ARG:HG3	2.02	0.40
3:N:45:PHE:O	3:N:86:ARG:NH2	2.54	0.40
3:N:890:VAL:HB	3:N:922:LEU:HD13	2.04	0.40
3:N:215:TYR:HE1	3:N:381:ALA:H	1.70	0.40
4:E:83:ASP:N	4:E:83:ASP:OD1	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	224/315 (71%)	222 (99%)	2 (1%)	0	100	100
1	B	220/315 (70%)	215 (98%)	5 (2%)	0	100	100
1	K	224/315 (71%)	222 (99%)	2 (1%)	0	100	100
1	L	223/315 (71%)	218 (98%)	5 (2%)	0	100	100
2	C	1107/1119 (99%)	1086 (98%)	21 (2%)	0	100	100
2	M	1107/1119 (99%)	1080 (98%)	27 (2%)	0	100	100
3	D	1482/1524 (97%)	1455 (98%)	26 (2%)	1 (0%)	56	87

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	N	1482/1524 (97%)	1454 (98%)	27 (2%)	1 (0%)	56 87
4	E	92/99 (93%)	89 (97%)	2 (2%)	1 (1%)	17 51
4	O	92/99 (93%)	90 (98%)	2 (2%)	0	100 100
5	F	344/443 (78%)	339 (98%)	5 (2%)	0	100 100
5	P	345/443 (78%)	341 (99%)	4 (1%)	0	100 100
All	All	6942/7630 (91%)	6811 (98%)	128 (2%)	3 (0%)	100 100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	E	94	PRO
3	D	530	VAL
3	N	530	VAL

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	199/273 (73%)	187 (94%)	12 (6%)	24 57
1	B	195/273 (71%)	185 (95%)	10 (5%)	29 65
1	K	199/273 (73%)	188 (94%)	11 (6%)	27 61
1	L	198/273 (72%)	191 (96%)	7 (4%)	43 78
2	C	936/941 (100%)	869 (93%)	67 (7%)	18 46
2	M	936/941 (100%)	870 (93%)	66 (7%)	18 47
3	D	1253/1279 (98%)	1166 (93%)	87 (7%)	19 48
3	N	1253/1279 (98%)	1169 (93%)	84 (7%)	20 50
4	E	83/88 (94%)	82 (99%)	1 (1%)	78 94
4	O	83/88 (94%)	82 (99%)	1 (1%)	78 94
5	F	301/388 (78%)	285 (95%)	16 (5%)	28 63
5	P	302/388 (78%)	269 (89%)	33 (11%)	8 23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	5938/6484 (92%)	5543 (93%)	395 (7%)	20 50

All (395) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	34	VAL
1	A	67	THR
1	A	104	GLU
1	A	126	ASP
1	A	142	VAL
1	A	184	THR
1	A	186	LEU
1	A	189	ARG
1	A	205	VAL
1	A	219	ARG
1	A	229	GLN
1	B	34	VAL
1	B	80	LEU
1	B	94	LEU
1	B	112	ARG
1	B	158	ILE
1	B	186	LEU
1	B	197	LEU
1	B	199	ILE
1	B	206	THR
1	B	215	VAL
2	C	8	ARG
2	C	11	GLU
2	C	15	LEU
2	C	56	GLU
2	C	81	ASP
2	C	97	ARG
2	C	103	LYS
2	C	107	LEU
2	C	133	ASP
2	C	141	HIS
2	C	168	ARG
2	C	177	GLU
2	C	205	GLU
2	C	221	LEU
2	C	232	GLU

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Mol	Chain	Res	Type
2	C	251	ASP
2	C	322	VAL
2	C	331	ARG
2	C	342	ASP
2	C	358	ARG
2	C	372	LEU
2	C	403	SER
2	C	418	LEU
2	C	427	VAL
2	C	434	HIS
2	C	454	SER
2	C	464	LEU
2	C	480	THR
2	C	482	GLU
2	C	512	ARG
2	C	524	VAL
2	C	557	ARG
2	C	575	GLN
2	C	583	LEU
2	C	586	ARG
2	C	589	ARG
2	C	591	SER
2	C	592	LEU
2	C	610	ARG
2	C	617	ASP
2	C	633	GLN
2	C	638	ASP
2	C	640	ARG
2	C	648	ARG
2	C	659	PRO
2	C	683	ASN
2	C	771	GLU
2	C	774	LEU
2	C	775	ARG
2	C	786	LYS
2	C	807	ARG
2	C	808	ARG
2	C	813	VAL
2	C	815	LEU
2	C	830	LYS
2	C	848	VAL
2	C	916	GLU

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Mol	Chain	Res	Type
2	C	923	GLU
2	C	928	LYS
2	C	939	ARG
2	C	942	GLU
2	C	952	LEU
2	C	968	LEU
2	C	978	ARG
2	C	1001	VAL
2	C	1014	SER
2	C	1057	SER
3	D	30	GLU
3	D	67	ARG
3	D	81	THR
3	D	106	LYS
3	D	135	LEU
3	D	141	ILE
3	D	155	ASP
3	D	161	LEU
3	D	190	GLU
3	D	191	LEU
3	D	198	ARG
3	D	200	ASP
3	D	204	LEU
3	D	230	TRP
3	D	231	VAL
3	D	256	GLU
3	D	272	LEU
3	D	275	GLU
3	D	276	ASP
3	D	312	ARG
3	D	325	GLU
3	D	331	VAL
3	D	335	LEU
3	D	362	GLU
3	D	372	ASP
3	D	387	LEU
3	D	399	ARG
3	D	411	THR
3	D	421	LEU
3	D	486	ARG
3	D	500	ARG
3	D	525	ARG

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Mol	Chain	Res	Type
3	D	548	ILE
3	D	572	ARG
3	D	576	GLU
3	D	587	ARG
3	D	591	VAL
3	D	610	LYS
3	D	618	LEU
3	D	632	VAL
3	D	646	LYS
3	D	650	LEU
3	D	669	ASN
3	D	709	HIS
3	D	754	PHE
3	D	778	LEU
3	D	808	THR
3	D	817	GLU
3	D	827	ILE
3	D	832	ARG
3	D	864	VAL
3	D	875	THR
3	D	894	LYS
3	D	904	VAL
3	D	943	THR
3	D	972	LEU
3	D	983	LEU
3	D	984	THR
3	D	1041	LEU
3	D	1062	ARG
3	D	1079	LYS
3	D	1083	ASP
3	D	1127	GLU
3	D	1128	VAL
3	D	1130	ARG
3	D	1155	VAL
3	D	1162	GLU
3	D	1188	VAL
3	D	1195	GLN
3	D	1208	ASP
3	D	1219	GLU
3	D	1221	VAL
3	D	1277	ILE
3	D	1284	GLU

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Mol	Chain	Res	Type
3	D	1287	GLU
3	D	1288	GLU
3	D	1290	LEU
3	D	1304	LYS
3	D	1305	LEU
3	D	1307	LYS
3	D	1313	VAL
3	D	1317	ASP
3	D	1455	LYS
3	D	1470	ARG
3	D	1493	LYS
3	D	1496	GLU
3	D	1501	GLU
4	E	50	THR
5	F	88	ILE
5	F	123	ASP
5	F	150	THR
5	F	172	ARG
5	F	186	HIS
5	F	205	ARG
5	F	208	SER
5	F	218	GLN
5	F	279	GLN
5	F	310	ILE
5	F	364	ARG
5	F	377	ASP
5	F	396	ARG
5	F	417	LYS
5	F	420	ASP
5	F	422	LEU
1	K	6	LEU
1	K	34	VAL
1	K	67	THR
1	K	104	GLU
1	K	112	ARG
1	K	142	VAL
1	K	184	THR
1	K	186	LEU
1	K	205	VAL
1	K	219	ARG
1	K	229	GLN
1	L	34	VAL

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Mol	Chain	Res	Type
1	L	62	LEU
1	L	80	LEU
1	L	158	ILE
1	L	186	LEU
1	L	206	THR
1	L	215	VAL
2	M	11	GLU
2	M	15	LEU
2	M	27	ARG
2	M	81	ASP
2	M	82	GLU
2	M	113	VAL
2	M	133	ASP
2	M	141	HIS
2	M	154	ARG
2	M	157	ARG
2	M	174	LEU
2	M	177	GLU
2	M	182	VAL
2	M	194	VAL
2	M	196	LEU
2	M	198	ARG
2	M	217	LEU
2	M	224	GLU
2	M	250	ARG
2	M	251	ASP
2	M	274	ARG
2	M	322	VAL
2	M	331	ARG
2	M	342	ASP
2	M	358	ARG
2	M	372	LEU
2	M	403	SER
2	M	409	ARG
2	M	418	LEU
2	M	427	VAL
2	M	434	HIS
2	M	454	SER
2	M	464	LEU
2	M	480	THR
2	M	482	GLU
2	M	512	ARG

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Mol	Chain	Res	Type
2	M	524	VAL
2	M	557	ARG
2	M	575	GLN
2	M	583	LEU
2	M	589	ARG
2	M	610	ARG
2	M	617	ASP
2	M	627	ARG
2	M	633	GLN
2	M	638	ASP
2	M	640	ARG
2	M	648	ARG
2	M	670	GLN
2	M	683	ASN
2	M	768	THR
2	M	813	VAL
2	M	815	LEU
2	M	830	LYS
2	M	848	VAL
2	M	916	GLU
2	M	923	GLU
2	M	928	LYS
2	M	939	ARG
2	M	942	GLU
2	M	952	LEU
2	M	968	LEU
2	M	978	ARG
2	M	1001	VAL
2	M	1014	SER
2	M	1057	SER
3	N	30	GLU
3	N	35	ARG
3	N	65	ARG
3	N	68	PHE
3	N	81	THR
3	N	87	ARG
3	N	106	LYS
3	N	135	LEU
3	N	141	ILE
3	N	155	ASP
3	N	161	LEU
3	N	190	GLU

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Mol	Chain	Res	Type
3	N	191	LEU
3	N	198	ARG
3	N	200	ASP
3	N	204	LEU
3	N	227	LEU
3	N	230	TRP
3	N	256	GLU
3	N	270	LEU
3	N	277	GLU
3	N	286	VAL
3	N	306	GLU
3	N	311	LEU
3	N	322	VAL
3	N	331	VAL
3	N	362	GLU
3	N	372	ASP
3	N	387	LEU
3	N	399	ARG
3	N	411	THR
3	N	421	LEU
3	N	486	ARG
3	N	500	ARG
3	N	525	ARG
3	N	548	ILE
3	N	572	ARG
3	N	576	GLU
3	N	587	ARG
3	N	591	VAL
3	N	618	LEU
3	N	646	LYS
3	N	650	LEU
3	N	669	ASN
3	N	709	HIS
3	N	754	PHE
3	N	778	LEU
3	N	808	THR
3	N	817	GLU
3	N	827	ILE
3	N	832	ARG
3	N	864	VAL
3	N	875	THR
3	N	894	LYS

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Mol	Chain	Res	Type
3	N	904	VAL
3	N	943	THR
3	N	971	LEU
3	N	976	GLN
3	N	984	THR
3	N	1001	GLU
3	N	1009	LYS
3	N	1020	LEU
3	N	1041	LEU
3	N	1055	VAL
3	N	1062	ARG
3	N	1067	VAL
3	N	1100	ASP
3	N	1128	VAL
3	N	1129	THR
3	N	1130	ARG
3	N	1188	VAL
3	N	1200	VAL
3	N	1208	ASP
3	N	1219	GLU
3	N	1277	ILE
3	N	1280	VAL
3	N	1283	ILE
3	N	1317	ASP
3	N	1359	GLN
3	N	1366	LYS
3	N	1408	ILE
3	N	1444	THR
3	N	1459	LEU
3	N	1492	LEU
4	O	50	THR
5	P	78	SER
5	P	90	GLN
5	P	120	THR
5	P	150	THR
5	P	151	LEU
5	P	186	HIS
5	P	222	ARG
5	P	264	MET
5	P	287	THR
5	P	309	LYS
5	P	347	GLN

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Mol	Chain	Res	Type
5	P	358	LEU
5	P	361	LEU
5	P	363	GLU
5	P	375	LEU
5	P	376	ILE
5	P	379	ARG
5	P	383	LEU
5	P	393	THR
5	P	398	ARG
5	P	406	ARG
5	P	409	LYS
5	P	410	TYR
5	P	411	HIS
5	P	412	GLU
5	P	414	ARG
5	P	415	THR
5	P	416	ARG
5	P	417	LYS
5	P	418	LEU
5	P	420	ASP
5	P	422	LEU
5	P	423	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
3	D	1172	HIS
3	D	1195	GLN
2	M	187	ASN
3	N	350	HIS
5	P	90	GLN

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

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 14 ligands modelled in this entry, 14 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	226/315 (71%)	-0.34	0 100 100	45, 63, 96, 118	0
1	B	222/315 (70%)	-0.20	2 (0%) 85 84	47, 77, 114, 137	0
1	K	226/315 (71%)	-0.26	0 100 100	49, 66, 97, 116	0
1	L	225/315 (71%)	-0.19	2 (0%) 85 84	51, 81, 118, 139	0
2	C	1111/1119 (99%)	-0.14	8 (0%) 89 88	32, 59, 111, 149	0
2	M	1111/1119 (99%)	-0.05	35 (3%) 51 43	34, 65, 129, 152	0
3	D	1486/1524 (97%)	-0.12	21 (1%) 78 76	29, 62, 120, 177	1 (0%)
3	N	1486/1524 (97%)	-0.14	25 (1%) 73 70	32, 64, 118, 178	1 (0%)
4	E	94/99 (94%)	-0.31	0 100 100	41, 64, 111, 121	0
4	O	94/99 (94%)	-0.38	0 100 100	45, 67, 112, 122	0
5	F	346/443 (78%)	-0.24	1 (0%) 94 94	37, 63, 108, 132	0
5	P	347/443 (78%)	-0.13	10 (2%) 55 49	42, 72, 139, 172	0
6	G	16/19 (84%)	-0.32	0 100 100	57, 84, 176, 182	0
6	Q	16/19 (84%)	-0.36	0 100 100	69, 93, 180, 182	0
7	H	24/27 (88%)	-0.35	0 100 100	54, 98, 145, 192	0
7	R	24/27 (88%)	-0.25	0 100 100	55, 112, 147, 199	0
All	All	7054/7722 (91%)	-0.15	104 (1%) 76 74	29, 65, 121, 199	2 (0%)

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	P	410	TYR	4.3
2	M	363	SER	4.2
5	P	411	HIS	4.1
3	D	144	GLY	4.0
3	N	1129	THR	3.9

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Mol	Chain	Res	Type	RSRZ
2	M	152	PRO	3.9
2	M	311	PHE	3.8
5	P	415	THR	3.8
3	N	1305	LEU	3.7
3	D	1252	ILE	3.7
2	C	365	ASP	3.6
2	C	219	GLN	3.6
3	N	1128	VAL	3.6
3	N	1253	THR	3.5
3	D	976	GLN	3.4
2	M	102	HIS	3.4
2	M	367	LEU	3.3
5	P	413	SER	3.3
3	D	1253	THR	3.3
2	M	365	ASP	3.3
2	M	191	PHE	3.2
2	M	211	LEU	3.2
3	D	1128	VAL	3.2
2	M	210	GLU	3.2
2	M	764	GLU	3.2
2	M	181	VAL	3.1
3	N	191	LEU	3.1
5	P	359	SER	3.1
3	N	1299	PHE	3.0
3	D	1319	VAL	2.9
3	D	982	PHE	2.9
2	C	366	SER	2.9
2	M	778	PHE	2.9
3	D	1502	ALA	2.9
3	N	1252	ILE	2.8
2	M	219	GLN	2.8
3	D	1499	ARG	2.7
2	M	199	VAL	2.7
2	M	254	VAL	2.7
2	M	207	LEU	2.7
3	D	973	GLN	2.7
3	D	1294	VAL	2.7
5	P	392	VAL	2.6
3	D	1131	SER	2.6
1	L	16	GLN	2.6
3	D	831	GLY	2.5
2	M	364	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
3	N	68	PHE	2.5
2	M	362	GLY	2.5
3	D	1129	THR	2.5
1	L	65	PHE	2.5
3	N	1313	VAL	2.5
5	P	138	SER	2.4
3	N	807	ALA	2.4
3	N	1292	VAL	2.4
3	N	1298	GLY	2.4
2	M	240	THR	2.4
2	M	221	LEU	2.4
3	N	1500	LYS	2.3
5	P	406	ARG	2.3
3	N	1308	GLU	2.3
3	N	1312	LEU	2.3
2	C	811	PRO	2.3
1	B	65	PHE	2.3
2	M	368	THR	2.3
2	C	650	ARG	2.3
3	D	380	GLU	2.3
2	M	217	LEU	2.2
3	N	976	GLN	2.2
5	F	423	ASP	2.2
1	B	157	GLY	2.2
3	D	310	LEU	2.2
3	D	1312	LEU	2.2
2	C	364	GLU	2.2
2	M	741	GLY	2.2
2	C	176	VAL	2.2
5	P	423	ASP	2.2
2	M	101	ILE	2.2
3	N	805	GLU	2.2
3	N	355	VAL	2.2
2	M	104	ASP	2.1
2	M	180	GLY	2.1
3	D	839	LEU	2.1
3	D	977	ALA	2.1
2	C	8	ARG	2.1
3	N	1294	VAL	2.1
3	N	1495	ILE	2.1
2	M	222	MET	2.1
2	M	621	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
3	N	177	ALA	2.1
3	D	1297	GLU	2.1
3	N	1319	VAL	2.1
2	M	177	GLU	2.0
2	M	616	GLU	2.0
2	M	220	GLY	2.0
5	P	409	LYS	2.0
3	N	378	ILE	2.0
3	N	1325	LEU	2.0
3	D	241	ILE	2.0
3	N	1290	LEU	2.0
2	M	108	ILE	2.0
2	M	158	TYR	2.0
2	M	226	VAL	2.0
2	M	175	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
8	MG	K	1001	1/1	0.90	0.46	18.86	67,67,67,67	0
8	MG	N	2004	1/1	0.91	0.45	4.04	66,66,66,66	0
8	MG	D	2004	1/1	0.96	0.48	3.60	66,66,66,66	0
9	ZN	D	2001	1/1	0.99	0.23	2.72	77,77,77,77	0
8	MG	B	2001	1/1	0.51	0.27	2.58	71,71,71,71	0
9	ZN	N	2001	1/1	0.99	0.14	-0.55	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
9	ZN	N	2002	1/1	0.99	0.09	-0.95	95,95,95,95	0
9	ZN	D	2002	1/1	0.99	0.10	-1.13	73,73,73,73	0
8	MG	F	2001	1/1	0.87	0.08	-2.38	63,63,63,63	0
8	MG	P	2001	1/1	0.93	0.09	-	71,71,71,71	0
8	MG	D	2003	1/1	0.97	0.30	-	32,32,32,32	0
8	MG	N	2003	1/1	0.98	0.37	-	38,38,38,38	0
8	MG	N	2005	1/1	0.92	0.15	-	67,67,67,67	0
8	MG	D	2005	1/1	0.88	0.13	-	71,71,71,71	0

6.5 Other polymers (i)

There are no such residues in this entry.