



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 04:22 PM UTC

PDB ID : 4G7H / pdb_00004g7h
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

<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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

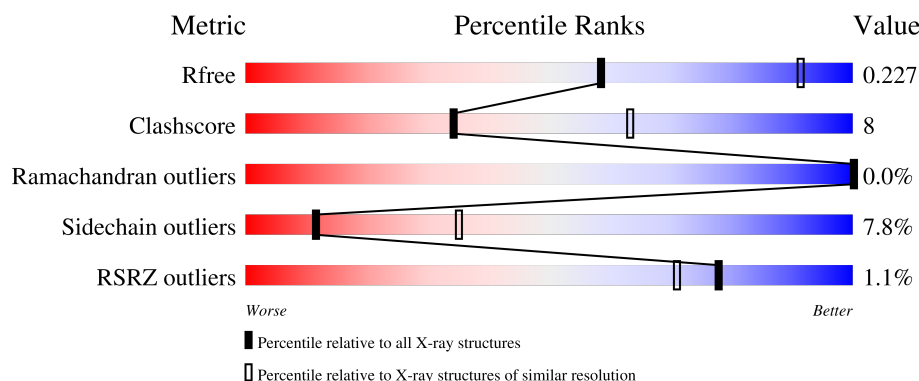
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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.



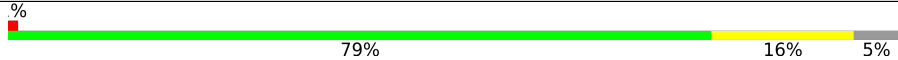
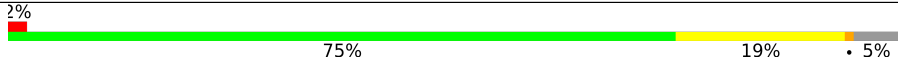
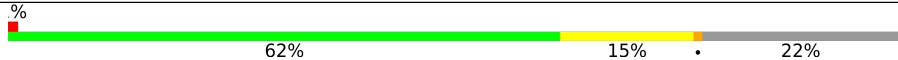
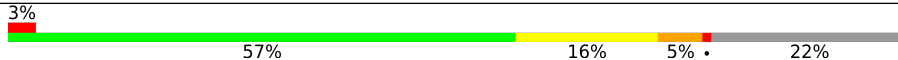
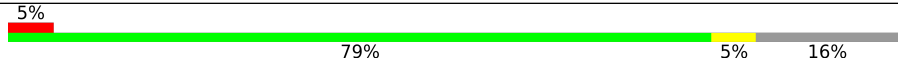
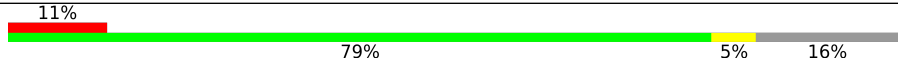
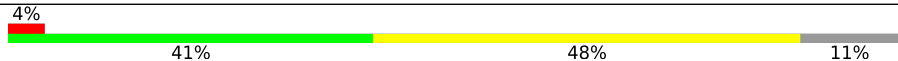
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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 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	% 53% 14% • 28%
1	B	315	3% 54% 13% • 30%
1	K	315	53% 16% • 28%
1	L	315	% 56% 14% • 29%
2	C	1119	% 76% 21% ••

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Mol	Chain	Length	Quality of chain
2	M	1119	
3	D	1524	
3	N	1524	
4	E	99	
4	O	99	
5	F	443	
5	P	443	
6	G	19	
6	Q	19	
7	H	27	
7	R	27	

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*C P*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 (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	K	1	Total	Mg	0	0
			1	1		
8	N	3	Total	Mg	0	0
			3	3		
8	P	1	Total	Mg	0	0
			1	1		

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

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

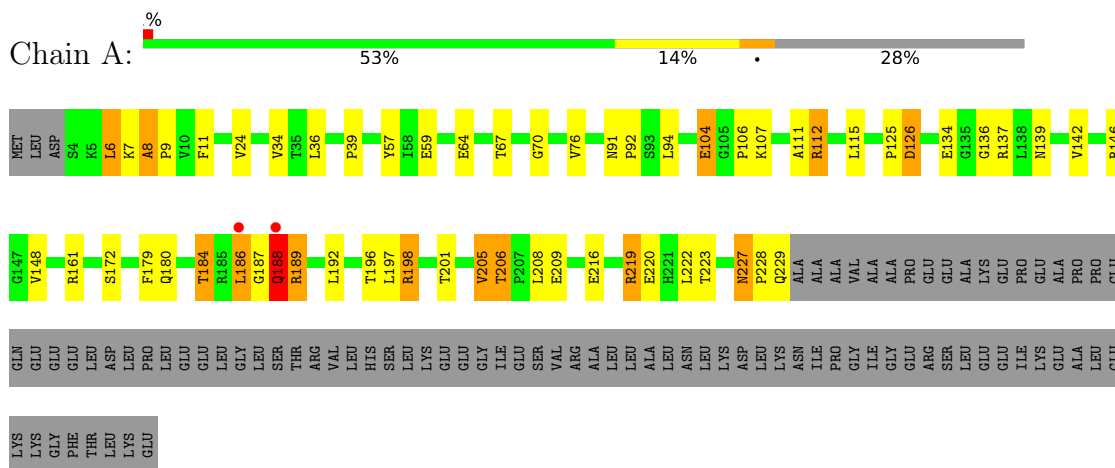
- Molecule 10 is water.

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

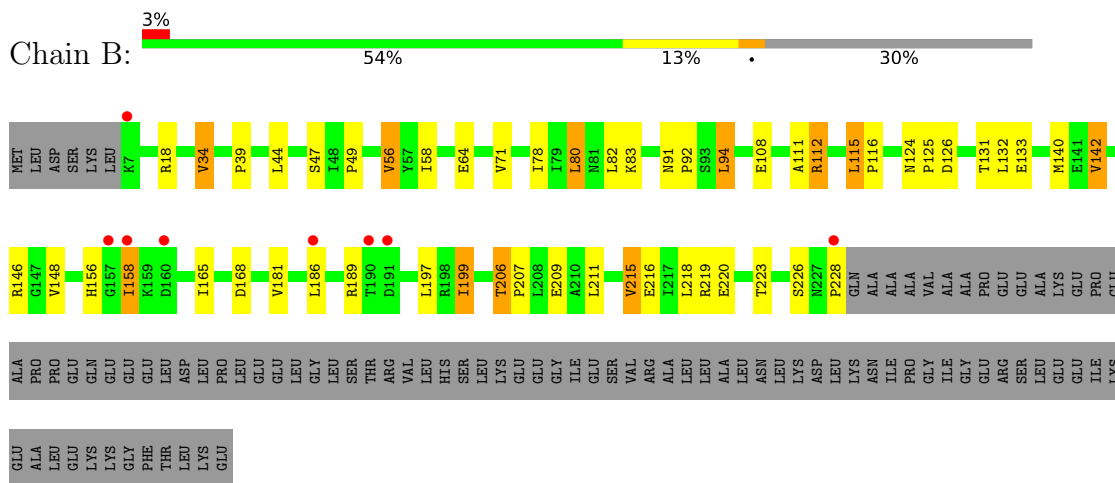
3 Residue-property plots

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

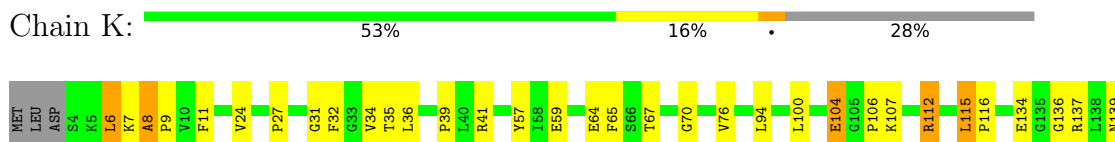
• Molecule 1: DNA-directed RNA polymerase subunit alpha

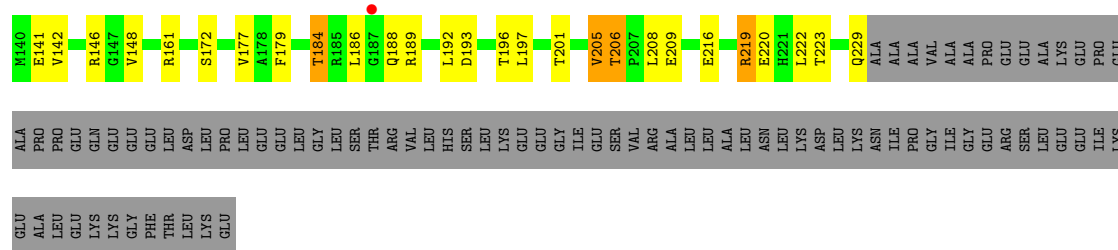


• Molecule 1: DNA-directed RNA polymerase subunit alpha

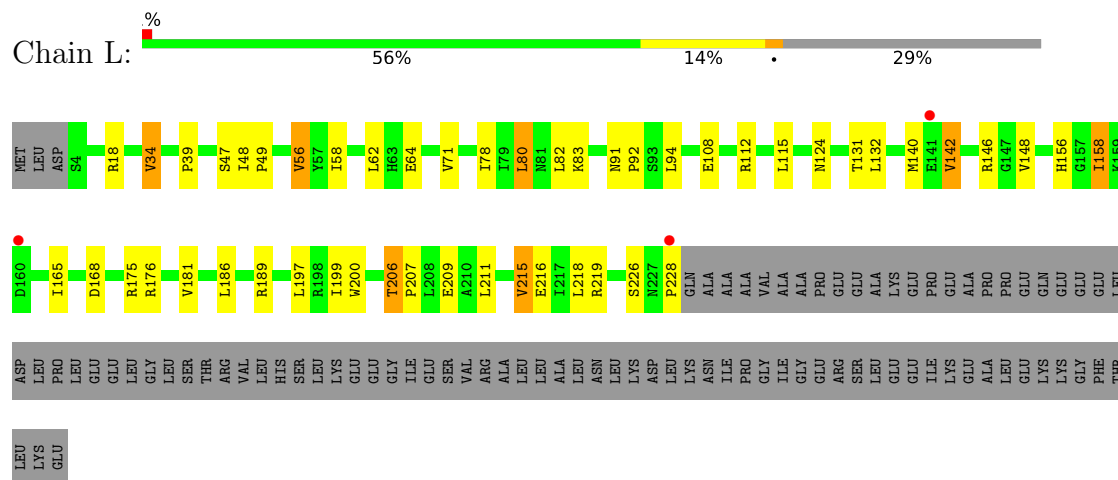


• Molecule 1: DNA-directed RNA polymerase subunit alpha

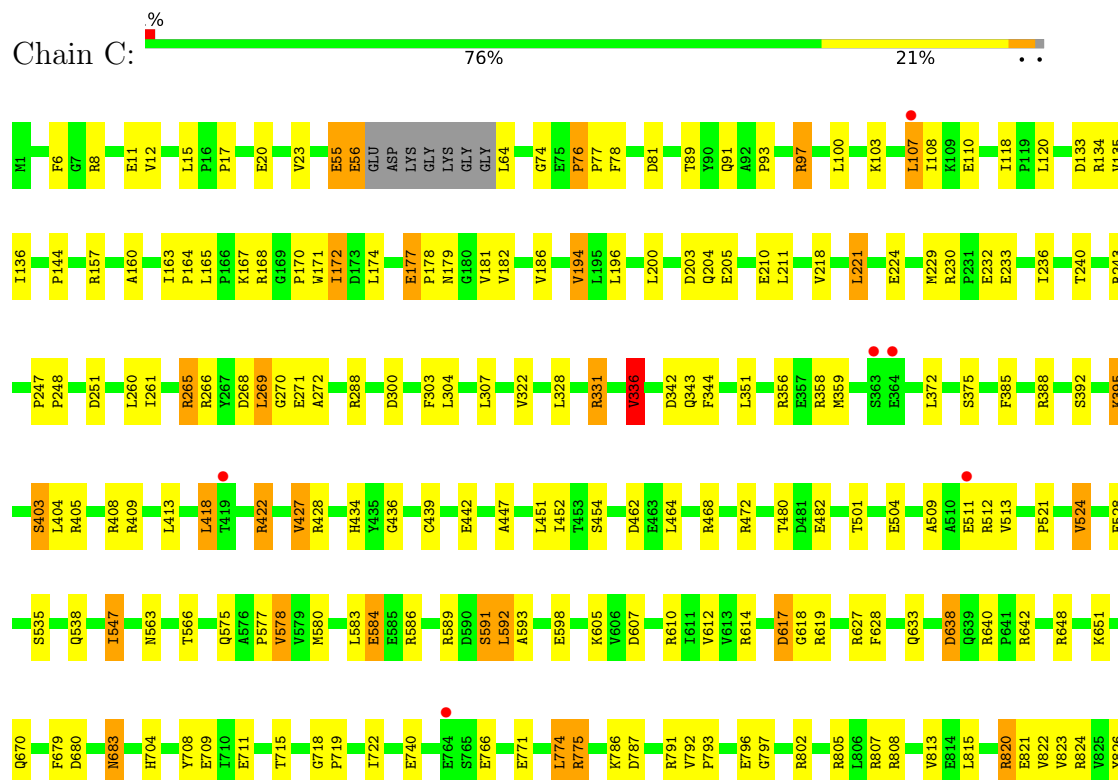


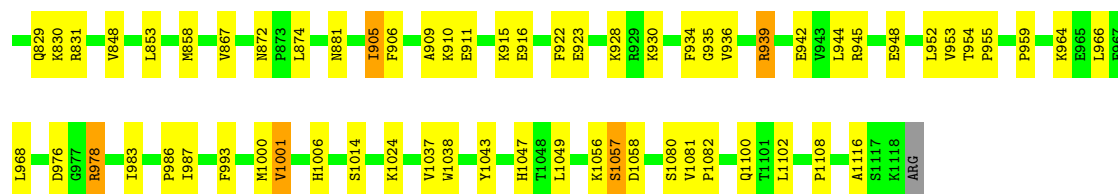


• Molecule 1: DNA-directed RNA polymerase subunit alpha

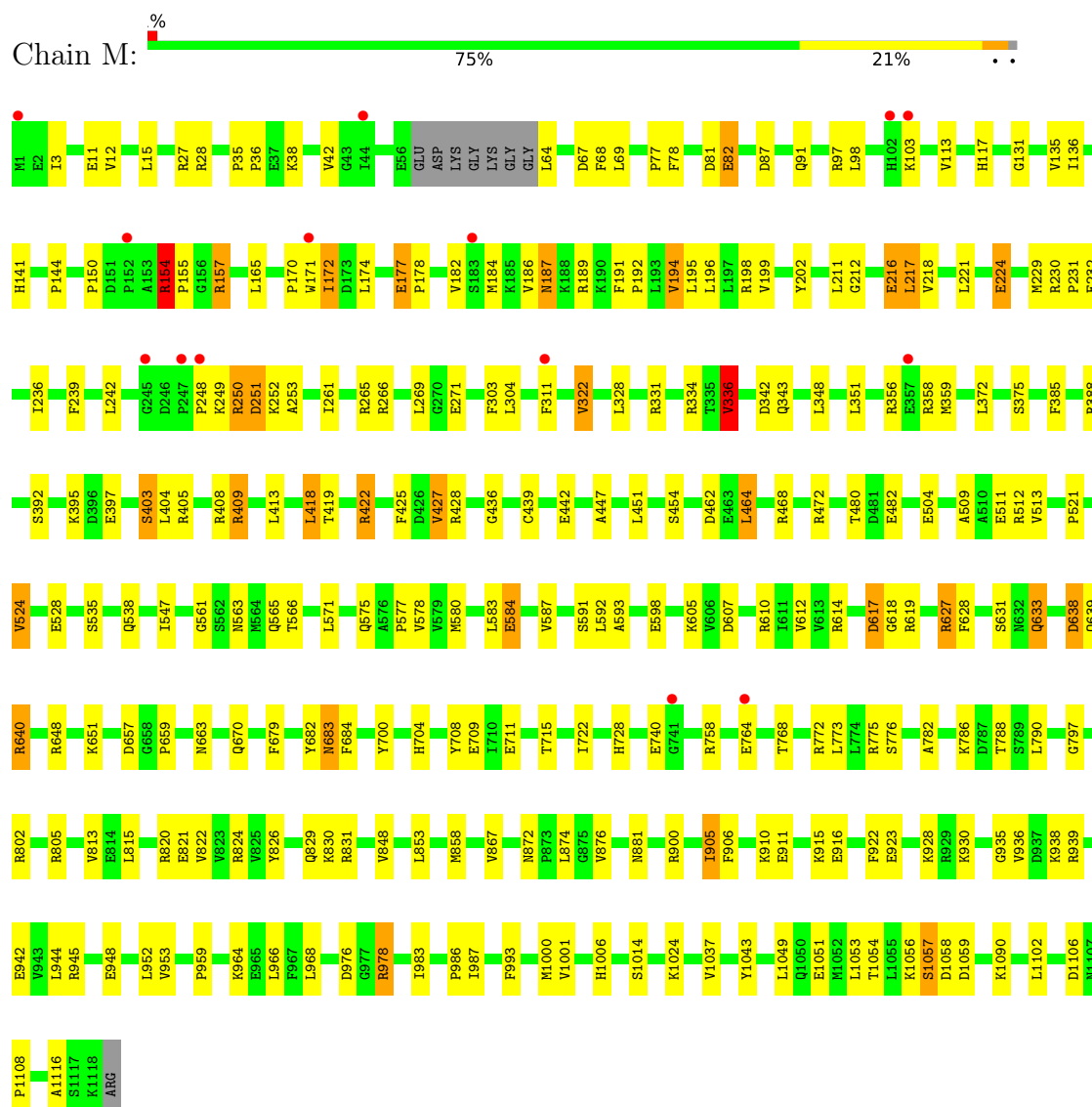


• Molecule 2: DNA-directed RNA polymerase subunit beta

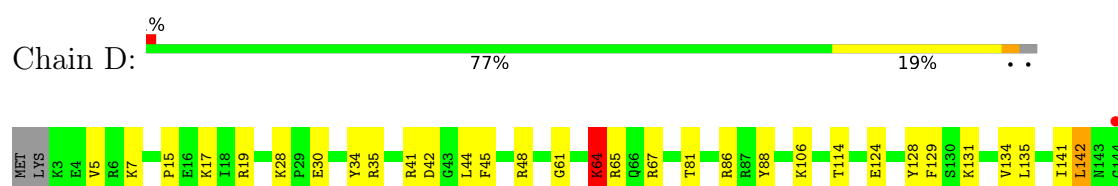


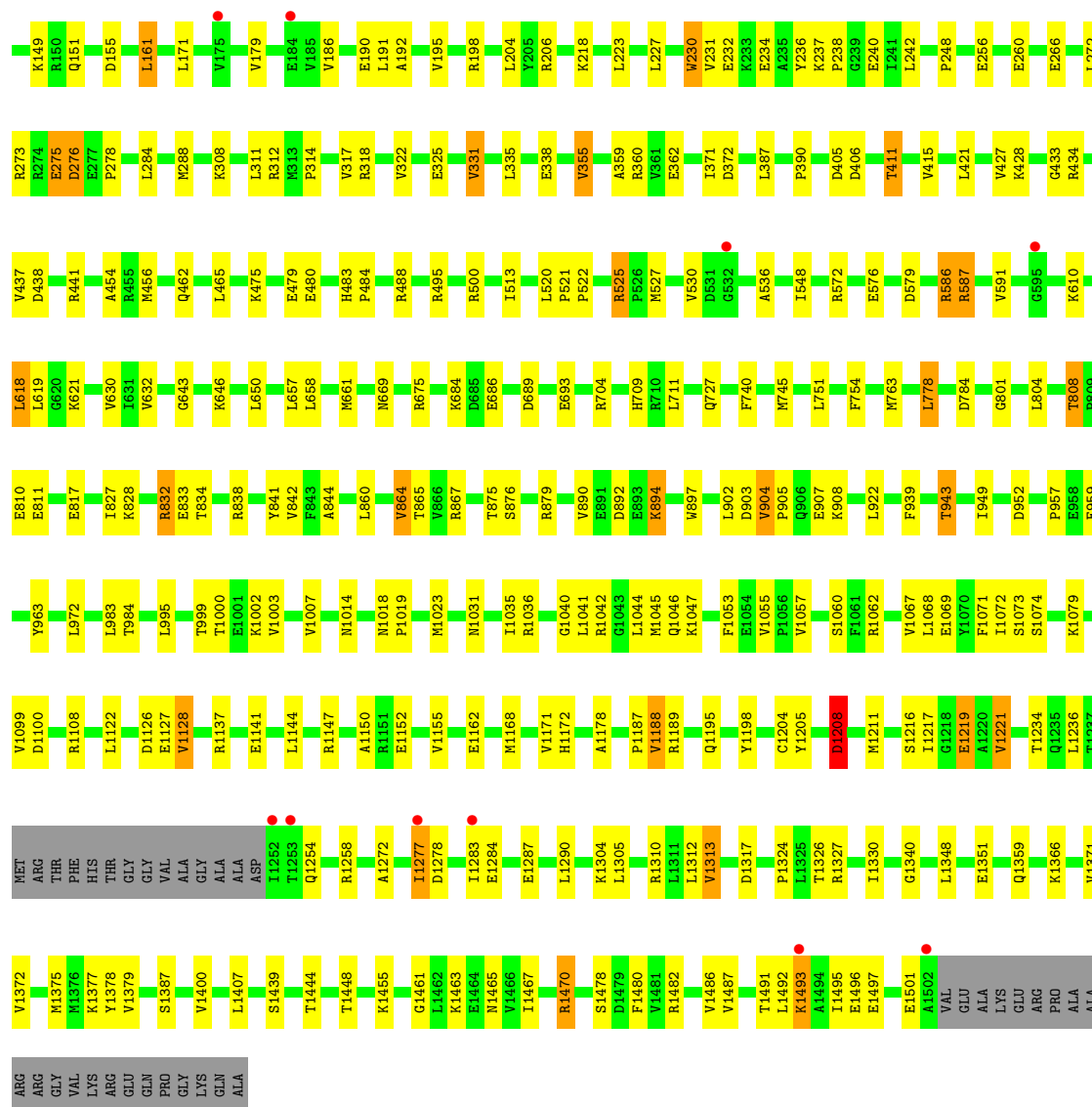


• Molecule 2: DNA-directed RNA polymerase subunit beta



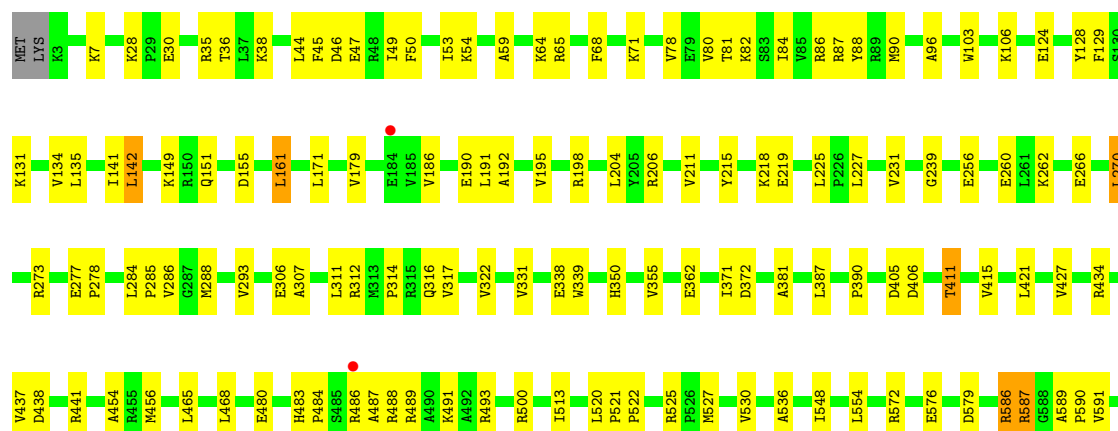
• Molecule 3: DNA-directed RNA polymerase subunit beta'

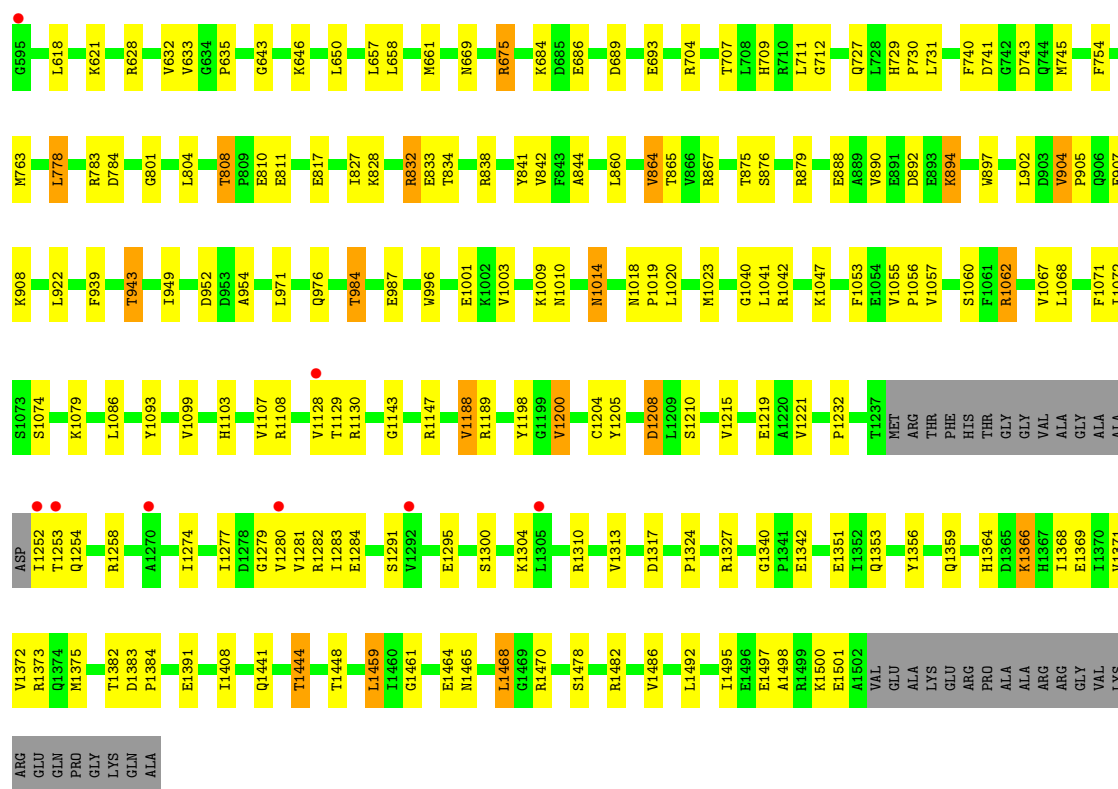




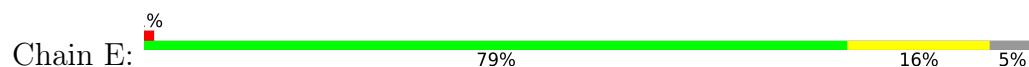
● Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain N: 77% 19% ..

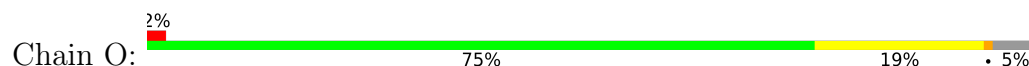




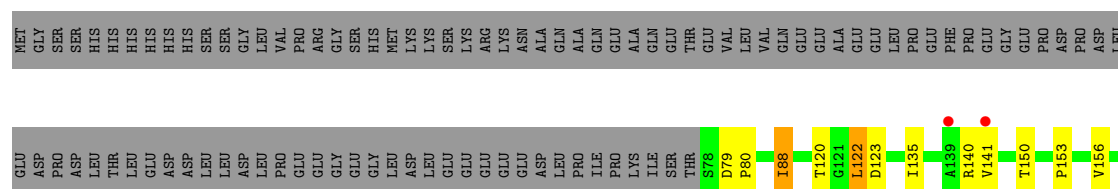
- Molecule 4: DNA-directed RNA polymerase subunit omega

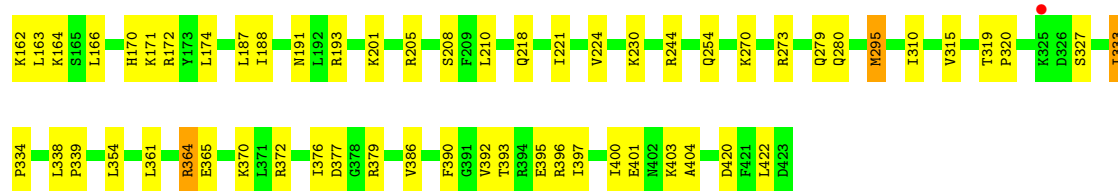


- Molecule 4: DNA-directed RNA polymerase subunit omega

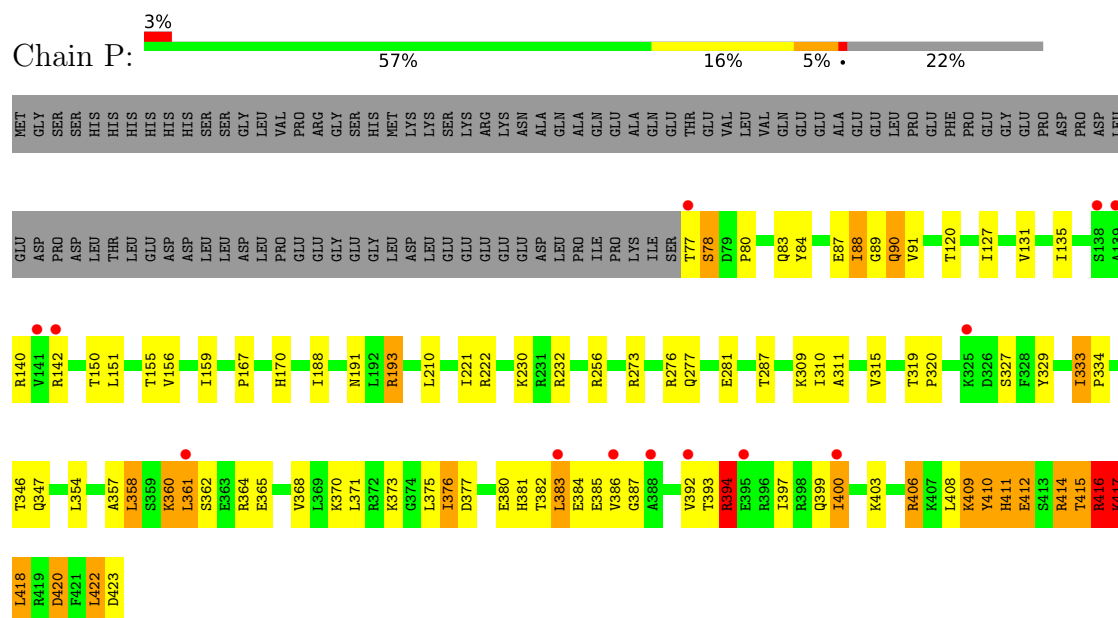


- Molecule 5: RNA polymerase sigma factor

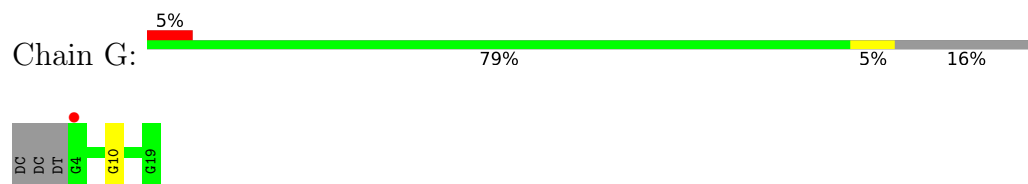




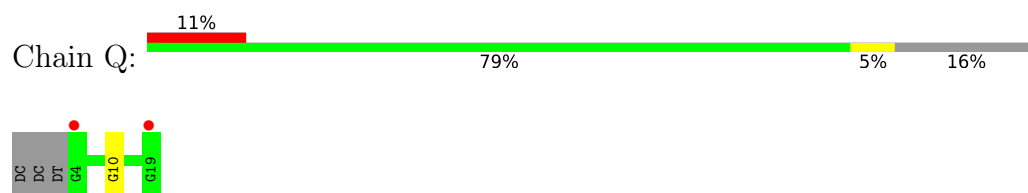
● Molecule 5: RNA polymerase sigma factor



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



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



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





● 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'



4 Data and refinement statistics

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 49.27 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.27-2.90) 99.6 (49.27-2.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.188 , 0.226 0.195 , 0.227	Depositor DCC
R_{free} test set	2205 reflections (0.88%)	wwPDB-VP
Wilson B-factor (Å ²)	61.5	Xtriage
Anisotropy	0.653	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.44	0/1814	0.94	12/2466 (0.5%)
1	B	0.39	0/1782	0.90	4/2424 (0.2%)
1	K	0.39	0/1814	0.90	8/2466 (0.3%)
1	L	0.38	0/1805	0.91	9/2454 (0.4%)
2	C	0.43	0/8937	0.85	24/12087 (0.2%)
2	M	0.41	0/8937	0.84	14/12087 (0.1%)
3	D	0.41	0/11944	0.82	13/16149 (0.1%)
3	N	0.41	0/11944	0.82	9/16149 (0.1%)
4	E	0.34	0/775	0.76	0/1045
4	O	0.36	0/775	0.74	0/1045
5	F	0.39	0/2852	0.82	5/3837 (0.1%)
5	P	0.40	0/2859	0.89	6/3847 (0.2%)
6	G	0.24	0/368	0.72	0/567
6	Q	0.19	0/368	0.74	0/567
7	H	0.25	0/556	0.84	0/858
7	R	0.22	0/556	0.82	0/858
All	All	0.40	0/58086	0.84	104/78906 (0.1%)

There are no bond length outliers.

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	P	417	LYS	N-CA-C	8.85	123.58	111.54
5	P	416	ARG	N-CA-C	8.15	121.68	108.32
1	L	112	ARG	NE-CZ-NH2	7.76	126.19	119.20
2	C	422	ARG	NE-CZ-NH2	7.60	126.04	119.20
1	A	187	GLY	N-CA-C	-7.50	105.47	115.21
2	M	154	ARG	CA-C-N	7.46	127.17	119.56
2	M	154	ARG	C-N-CA	7.46	127.17	119.56
3	N	1340	GLY	CA-C-N	7.39	126.65	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	1340	GLY	C-N-CA	7.39	126.65	118.97
2	M	422	ARG	CD-NE-CZ	7.26	134.57	124.40
1	L	112	ARG	NE-CZ-NH1	-7.24	114.26	121.50
2	C	422	ARG	NE-CZ-NH1	-7.17	114.33	121.50
5	P	191	ASN	N-CA-C	7.16	121.73	112.92
3	N	28	LYS	CA-C-N	6.88	126.57	119.82
3	N	28	LYS	C-N-CA	6.88	126.57	119.82
2	C	269	LEU	N-CA-C	-6.71	101.67	110.53
2	M	271	GLU	N-CA-C	-6.67	104.08	111.36
2	C	271	GLU	N-CA-C	-6.67	104.09	111.36
2	C	170	PRO	CA-C-N	-6.59	110.81	122.07
2	C	170	PRO	C-N-CA	-6.59	110.81	122.07
1	A	198	ARG	NE-CZ-NH1	-6.55	114.95	121.50
1	A	198	ARG	NE-CZ-NH2	6.48	125.03	119.20
2	M	422	ARG	NE-CZ-NH2	-6.42	113.42	119.20
1	A	172	SER	CA-C-N	6.40	126.02	119.56
1	A	172	SER	C-N-CA	6.40	126.02	119.56
2	M	170	PRO	CA-C-N	-6.38	111.17	122.07
2	M	170	PRO	C-N-CA	-6.38	111.17	122.07
2	M	269	LEU	N-CA-C	-6.34	102.17	110.53
2	C	170	PRO	CA-C-O	-6.32	114.29	122.12
2	M	303	PHE	N-CA-C	6.27	118.63	111.11
3	D	1340	GLY	CA-C-N	6.10	125.31	118.97
3	D	1340	GLY	C-N-CA	6.10	125.31	118.97
2	C	303	PHE	N-CA-C	6.10	118.43	111.11
1	K	172	SER	CA-C-N	6.01	125.63	119.56
1	K	172	SER	C-N-CA	6.01	125.63	119.56
5	F	333	ILE	CA-C-N	6.00	125.97	120.03
5	F	333	ILE	C-N-CA	6.00	125.97	120.03
3	D	64	LYS	N-CA-C	5.98	120.70	113.17
1	A	188	GLN	N-CA-C	-5.91	105.73	113.12
2	C	422	ARG	CD-NE-CZ	5.85	132.59	124.40
3	D	1313	VAL	N-CA-C	5.85	116.36	108.17
2	C	336	VAL	CB-CA-C	-5.82	104.43	111.88
3	D	28	LYS	CA-C-N	5.76	125.86	119.87
3	D	28	LYS	C-N-CA	5.76	125.86	119.87
2	M	439	CYS	CA-C-N	5.74	125.35	119.56
2	M	439	CYS	C-N-CA	5.74	125.35	119.56
5	P	394	ARG	N-CA-C	5.71	117.58	111.36
2	C	23	VAL	N-CA-C	5.67	116.32	110.36
1	K	8	ALA	CA-C-N	5.65	125.84	120.31
1	K	8	ALA	C-N-CA	5.65	125.84	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	47	SER	N-CA-C	5.64	120.28	113.17
1	A	8	ALA	CA-C-N	5.64	125.83	120.31
1	A	8	ALA	C-N-CA	5.64	125.83	120.31
3	N	740	PHE	N-CA-C	5.62	119.12	112.72
3	N	1279	GLY	N-CA-C	5.62	118.16	110.69
5	F	191	ASN	N-CA-C	5.61	119.82	112.92
3	D	1208	ASP	N-CA-C	-5.57	99.44	108.41
1	L	47	SER	N-CA-C	5.56	120.18	113.17
5	F	327	SER	N-CA-C	5.54	117.82	109.23
3	N	64	LYS	N-CA-C	5.49	120.09	113.17
1	A	115	LEU	CA-C-N	5.47	125.39	119.76
1	A	115	LEU	C-N-CA	5.47	125.39	119.76
2	M	422	ARG	NE-CZ-NH1	5.45	126.95	121.50
2	M	336	VAL	CB-CA-C	-5.45	104.91	111.88
1	L	226	SER	N-CA-C	5.41	117.04	111.03
2	C	422	ARG	CG-CD-NE	5.41	123.91	112.00
1	B	226	SER	N-CA-C	5.36	116.98	111.03
1	L	112	ARG	CD-NE-CZ	5.32	131.85	124.40
2	C	593	ALA	N-CA-C	5.30	116.74	111.07
3	D	129	PHE	N-CA-C	5.29	118.88	111.74
2	C	439	CYS	CA-C-N	5.26	124.87	119.56
2	C	439	CYS	C-N-CA	5.26	124.87	119.56
3	D	65	ARG	N-CA-C	5.25	116.97	109.14
1	K	112	ARG	NE-CZ-NH2	-5.23	114.50	119.20
5	P	327	SER	N-CA-C	5.22	117.12	109.24
2	C	55	GLU	N-CA-C	5.21	118.10	111.69
2	C	388	ARG	N-CA-C	5.21	119.74	113.17
2	C	501	THR	CA-C-N	5.21	125.12	119.76
2	C	501	THR	C-N-CA	5.21	125.12	119.76
5	F	254	GLN	N-CA-C	5.20	119.77	113.38
1	A	227	ASN	CA-C-N	5.18	125.65	120.52
1	A	227	ASN	C-N-CA	5.18	125.65	120.52
3	N	1014	ASN	N-CA-C	5.17	119.87	113.50
3	D	740	PHE	N-CA-C	5.16	118.61	112.72
1	K	115	LEU	CA-C-N	5.16	125.08	119.76
1	K	115	LEU	C-N-CA	5.16	125.08	119.76
3	D	751	LEU	N-CA-C	5.14	117.67	111.40
2	C	547	ILE	N-CA-C	5.14	112.64	107.55
2	C	718	GLY	CA-C-N	5.13	124.89	119.76
2	C	718	GLY	C-N-CA	5.13	124.89	119.76
2	M	388	ARG	N-CA-C	5.13	119.63	113.17
5	P	333	ILE	N-CA-C	5.13	113.57	107.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	115	LEU	CA-C-N	5.11	125.11	119.90
1	L	115	LEU	C-N-CA	5.11	125.11	119.90
1	B	115	LEU	CA-C-N	5.09	125.09	119.90
1	B	115	LEU	C-N-CA	5.09	125.09	119.90
3	D	433	GLY	N-CA-C	5.09	118.00	110.42
3	N	129	PHE	N-CA-C	5.04	118.55	111.74
2	C	76	PRO	CA-C-N	5.03	124.81	119.28
2	C	76	PRO	C-N-CA	5.03	124.81	119.28
1	L	48	ILE	CA-C-N	5.03	125.26	119.83
1	L	48	ILE	C-N-CA	5.03	125.26	119.83
3	D	1014	ASN	N-CA-C	5.03	119.56	113.38
1	K	112	ARG	CD-NE-CZ	5.01	131.42	124.40

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	40	0
1	B	1750	0	1797	33	0
1	K	1782	0	1834	35	0
1	L	1773	0	1826	27	0
2	C	8770	0	8874	148	0
2	M	8770	0	8874	165	0
3	D	11738	0	11971	163	0
3	N	11738	0	11971	165	0
4	E	761	0	778	11	0
4	O	761	0	778	13	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	2	0
10	N	89	0	0	3	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	864	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 8.

All (864) 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
2:M:172:ILE:CG1	2:M:186:VAL:HG22	1.96	0.95
5:P:415:THR:CG2	5:P:416:ARG:NE	2.30	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:NE2	5:P:90:GLN:CA	2.38	0.86
1:A:112:ARG:HG2	1:A:112:ARG:HH21	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:HD3	5:P:414:ARG:N	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:1254:GLN:HB3	3:N:1258:ARG:HB2	1.68	0.75
3:N:1310:ARG:HB2	3:N:1327: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
3:D:1208:ASP:OD1	3:D:1208:ASP:C	2.31	0.74
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:C:462:ASP:HB3	2:C:468:ARG:HD2	1.72	0.72
2:M:428:ARG:NH2	2:M:447:ALA:O	2.21	0.72
2:C:1056:LYS:NZ	10:C:1208:HOH:O	2.21	0.72
2:M:983:ILE:HG21	2:M:987:ILE:HD11	1.70	0.72
2:C:853:LEU:HB2	2:C:858:MET:HE1	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:709:GLU:OE2	2:C:824:ARG:NH1	2.22	0.72
5:P:417:LYS:O	5:P:417:LYS:CG	2.32	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:HH21	1:A:112:ARG:CG	1.99	0.71
3:D:218:LYS:HG2	3:D:338:GLU:HG2	1.71	0.71
3:N:1208:ASP:C	3:N:1208:ASP:OD1	2.30	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
2:C:983:ILE:HG21	2:C:987:ILE:HD11	1.72	0.71
5:F:188:ILE:HD13	5:F:221:ILE:HG12	1.73	0.71
3:N:657:LEU:HG	3:N:661:MET:HE2	1.73	0.71
2:M:853:LEU:HB2	2:M:858:MET:HE1	1.73	0.70
3:D:657:LEU:HG	3:D:661:MET:HE2	1.73	0.70
3:N:633:VAL:HG13	3:N:633:VAL:O	1.91	0.70
2:M:172:ILE:HG13	2:M:186:VAL:CG2	2.11	0.70
2:M:773:LEU:HD23	5:P:354:LEU:HD13	1.74	0.69
1:K:193:ASP:OD2	2:M:938:LYS:NZ	2.19	0.69
2:M:144:PRO:HG2	2:M:165:LEU:HD23	1.74	0.69
3:D:142:LEU:HB2	3:D:161:LEU:HD11	1.73	0.69
3:N:520:LEU:O	3:N:525:ARG:NH1	2.25	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:D:520:LEU:O	3:D:525:ARG:NH1	2.26	0.68
3:D:1372:VAL:HA	3:D:1375:MET:HE3	1.76	0.68
2:M:1059:ASP:OD1	2:M:1059:ASP:C	2.36	0.68
3:N:142:LEU:HB2	3:N:161:LEU:HD11	1.74	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:124:GLU:OE2	3:N:587:ARG:NH2	2.28	0.67
3:N:36:THR:HG23	3:N:38:LYS:H	1.59	0.67
5:P:273:ARG:HG2	5:P:276:ARG:HH12	1.58	0.67
3:D:260:GLU:OE1	3:D:273:ARG:NH1	2.24	0.67
2:C:266:ARG:NH1	7:H:11:DG:N7	2.43	0.66
3:D:949:ILE:HD11	3:D:1023:MET:HE1	1.76	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:H	5:P:383:LEU:HD22	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:C:55:GLU:O	2:C:56:GLU:HB3	1.97	0.64
2:M:776:SER:OG	5:P:373:LYS:NZ	2.27	0.64
3:D:284:LEU:HD22	3:D:288:MET:HE2	1.80	0.64
3:N:1258:ARG:HH21	3:N:1351:GLU:HG2	1.63	0.64
5:P:414:ARG:N	5:P:414:ARG:CD	2.61	0.64
2:C:164:PRO:HD2	2:C:171:TRP:CD1	2.33	0.63
3:D:371:ILE:HG23	5:F:230:LYS:HD2	1.79	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:N:1371:VAL:HG12	3:N:1375:MET:HE2	1.79	0.63
3:D:1495:ILE:HG12	4:E:88:GLU:HG3	1.80	0.63
5:P:89:GLY:C	5:P:90:GLN:HE21	2.05	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
5:P:415:THR:C	5:P:416:ARG:HG3	2.17	0.62
2:C:708:TYR:OH	2:C:796:GLU:OE1	2.18	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
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
2:C:711:GLU:HG2	2:C:822:VAL:HG22	1.82	0.60
5:P:415:THR:CG2	5:P:416:ARG:HE	2.13	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
1:K:222:LEU:HD22	1:L:215:VAL:HG12	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1491:THR:HG21	4:E:89:MET:HG2	1.83	0.60
2:M:141:HIS:CE1	2:M:334:ARG:HD2	2.37	0.60
1:K:104:GLU:OE2	1:K:137:ARG:NH1	2.35	0.60
2:M:704:HIS:CE1	2:M:1000:MET:HE1	2.37	0.60
2:C:211:LEU:HD11	2:C:304:LEU:HD11	1.82	0.59
2:M:184:MET:HE3	2:M:186:VAL:HG21	1.84	0.59
1:A:24:VAL:HG22	1:A:196:THR:HG23	1.83	0.59
2:M:171:TRP:CE3	7:R:13:DT:H2'	2.37	0.59
7:H:5:DA:N6	10:H:101:HOH:O	2.35	0.59
1:K:216:GLU:OE2	1:K:219:ARG:NH2	2.36	0.59
7:R:12:DC:H1'	7:R:13:DT:C5	2.37	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
1:A:106:PRO:HG3	1:A:134:GLU:HG2	1.85	0.58
2:C:243:ARG:NH2	7:H:9:DG:O6	2.22	0.58
5:P:167:PRO:HG2	5:P:170:HIS:HB2	1.85	0.58
2:C:802:ARG:HB2	2:C:826:TYR:HB2	1.85	0.58
1:B:112:ARG:NH1	1:B:126:ASP:CG	2.62	0.58
2:M:409:ARG:HG2	2:M:409:ARG:HH11	1.68	0.58
3:D:1071:PHE:O	3:D:1074:SER:OG	2.22	0.58
5:F:361:LEU:HB3	5:F:365:GLU:HG3	1.85	0.58
1:A:198:ARG:HD3	2:C:934:PHE:CZ	2.37	0.58
2:C:766:GLU:HG3	3:D:64:LYS:HD2	1.85	0.58
1:A:222:LEU:HD22	1:B:215:VAL:HG12	1.85	0.58
5:P:412:GLU:O	5:P:416:ARG:HD2	2.03	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
2:C:422:ARG:HG2	7:H:15:DT:OP2	2.04	0.57
3:N:262:LYS:NZ	10:N:2131:HOH:O	2.37	0.57
5:P:360:LYS:NZ	5:P:416:ARG:HH22	2.02	0.57
2:M:617:ASP:OD1	2:M:617:ASP:N	2.38	0.57
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
2:M:683:ASN:HB3	2:M:872:ASN:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:949:ILE:HD11	3:N:1023:MET:HE1	1.87	0.56
3:D:134:VAL:HG12	3:D:454:ALA:HB2	1.88	0.56
5:F:393:THR:HG22	5:F:395:GLU:H	1.69	0.56
1:K:64:GLU:HG2	1:K:76:VAL:HG22	1.88	0.56
2:M:177:GLU:HG3	2:M:178:PRO:HD2	1.88	0.56
3:D:828:LYS:HG2	3:D:833:GLU:HB3	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
2:C:704:HIS:CE1	2:C:1000:MET:HE1	2.41	0.55
2:M:577:PRO:HG2	2:M:580:MET:HG2	1.87	0.55
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: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
2:C:136:ILE:HB	2:C:336:VAL:HG13	1.87	0.55
1:K:222:LEU:HD21	1:L:218:LEU:HD23	1.88	0.55
3:D:841:TYR:HB2	3:D:864:VAL:HG22	1.89	0.55
1:L:83:LYS:HE2	1:L:168:ASP:HB2	1.88	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
3:D:434:ARG:NH2	5:F:135:ILE:O	2.40	0.54
1:L:80:LEU:HG	3:N:844:ALA:HA	1.90	0.54
2:M:418:LEU:HD21	2:M:427:VAL:HG11	1.89	0.54
5:P:415:THR:HB	5:P:416:ARG:HE	1.72	0.54
2:C:617:ASP:HB2	2:C:619:ARG:HG2	1.89	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:C:177:GLU:HG3	2:C:178:PRO:HD2	1.89	0.54
2:M:3:ILE:HD13	2:M:900:ARG:HB2	1.90	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)
3:N:90:MET:HE3	3:N:520:LEU:HA	1.90	0.54
2:M:212:GLY:HA2	2:M:218:VAL:HG11	1.90	0.54
2:M:607:ASP:HB2	2:M:610:ARG:NH1	2.23	0.54
5:P:418:LEU:O	5:P:418:LEU:HD23	2.08	0.54
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:C:577:PRO:HG2	2:C:580:MET:HG2	1.89	0.53
2:M:627:ARG:NH1	2:M:638:ASP:OD2	2.41	0.53
3:N:239:GLY:O	3:N:312:ARG:NH2	2.40	0.53
2:C:607:ASP:HB2	2:C:610:ARG:NH1	2.24	0.53
2:M:136:ILE:HB	2:M:336:VAL:HG13	1.90	0.53
2:M:617:ASP:HB2	2:M:619:ARG:HG2	1.89	0.53
2:M:628:PHE:H	2:M:638:ASP:CB	2.20	0.53
3:N:1497:GLU:HA	3:N:1500:LYS:HB2	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:658:LEU:HA	3:N:661:MET:HE3	1.91	0.53
3:D:1150:ALA:HB3	3:D:1187:PRO:HB2	1.90	0.53
3:N:90:MET:HG2	3:N:521:PRO:HD3	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
3:D:904:VAL:HG22	3:D:905:PRO:HD2	1.90	0.53
2:M:521:PRO:HB3	3:N:1068:LEU:HD21	1.90	0.53
2:M:1006:HIS:HB2	2:M:1024:LYS:HG3	1.90	0.53
2:C:1058:ASP:OD2	3:D:621:LYS:HE2	2.09	0.53
3:D:44:LEU:HB3	3:D:525:ARG:NH2	2.24	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
5:F:270:LYS:HE2	5:F:295:MET:HE1	1.90	0.53
1:B:83:LYS:HE2	1:B:168:ASP:HB2	1.90	0.53
2:M:217:LEU:HD13	2:M:217:LEU:H	1.74	0.53
2:M:1106:ASP:OD1	3:N:7:LYS:NZ	2.25	0.53
3:N:633:VAL:O	3:N:633:VAL:CG1	2.57	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
1:L:71:VAL:HG22	1:L:132:LEU:HG	1.92	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
3:N:1093:TYR:OH	3:N:1441:GLN:OE1	2.19	0.52
1:A:57:TYR:CD1	1:A:161:ARG:HD2	2.45	0.52
1:B:111:ALA:HB3	1:B:125:PRO:CA	2.36	0.52
5:F:153:PRO:HA	5:F:156:VAL:HG22	1.91	0.52
4:O:45:ARG:NH1	4:O:56:ASP:OD2	2.42	0.52
2:C:418:LEU:HD21	2:C:427:VAL:HG11	1.90	0.52
2:C:547:ILE:O	2:C:905:ILE:HD11	2.09	0.52
3:D:242:LEU:HB3	3:D:311:LEU:HD12	1.91	0.52
1:A:94:LEU:O	1:A:146:ARG:NH1	2.43	0.52
1:A:220:GLU:O	1:A:223:THR:HB	2.09	0.52
1:L:80:LEU:HB3	3:N:867:ARG:NH2	2.24	0.52
3:N:1274:ILE:HG22	3:N:1324:PRO:HA	1.92	0.52
2:M:704:HIS:CD2	2:M:831:ARG:HD2	2.44	0.52
3:N:1147:ARG:HD3	3:N:1188:VAL:HG11	1.91	0.52
3:N:411:THR:HB	3:N:437:VAL:H	1.75	0.52
3:N:1497:GLU:O	3:N:1501:GLU:HG2	2.10	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
3:D:1444:THR:O	3:D:1448:THR:HG23	2.09	0.52
3:N:904:VAL:HG22	3:N:905:PRO:HD2	1.91	0.52
5:P:415:THR:CB	5:P:416:ARG:HE	2.23	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
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:OE1	3:D:1046:GLN:N	2.40	0.51
3:N:1498:ALA:HB1	4:O:84:ARG:NH2	2.24	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
5:P:387:GLY:HA2	5:P:397:ILE:HD12	1.91	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
1:A:186:LEU:C	1:A:188:GLN:H	2.18	0.51
1:K:94:LEU:O	1:K:146:ARG:NH1	2.44	0.51
5:P:412:GLU:HA	5:P:416:ARG:CZ	2.40	0.51
1:A:206:THR:HB	1:A:209:GLU:HG3	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
2:C:1006:HIS:HB2	2:C:1024:LYS:HG3	1.91	0.51
3:D:192:ALA:HB3	3:D:195:VAL:HB	1.93	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
3:N:171:LEU:HD22	3:N:390:PRO:HG2	1.90	0.51
5:P:127:ILE:O	5:P:131:VAL:HG23	2.11	0.51
5:P:408:LEU:O	5:P:412:GLU:HB2	2.10	0.51
3:N:192:ALA:HB3	3:N:195:VAL:HB	1.93	0.51
3:N:1189:ARG:HB3	3:N:1204:CYS:HA	1.93	0.51
5:F:400:ILE:HG22	5:F:403:LYS:HE2	1.91	0.51
3:D:658:LEU:HA	3:D:661:MET:HE3	1.93	0.51
3:D:1208:ASP:OD2	3:D:1211:MET:HE2	2.11	0.51
2:M:605:LYS:HB2	2:M:612:VAL:HB	1.93	0.51
3:D:1258:ARG:HH21	3:D:1351:GLU:HG2	1.75	0.50
2:M:547:ILE:O	2:M:905:ILE:HD11	2.11	0.50
2:C:580:MET:HB3	2:C:584:GLU:CD	2.36	0.50
3:D:5:VAL:O	3:D:1470:ARG:NH2	2.44	0.50
3:D:1045:MET:HE2	3:D:1073:SER:HA	1.94	0.50
2:M:708:TYR:HB3	2:M:790:LEU:HD21	1.92	0.50
3:N:897:TRP:CH2	3:N:902:LEU:HD22	2.46	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
2:C:704:HIS:CD2	2:C:831:ARG:HD2	2.47	0.50
3:D:1053:PHE:CZ	3:D:1072:ILE:HD12	2.46	0.50
2:M:191:PHE:HB2	2:M:192:PRO:HD2	1.93	0.50
3:N:131:LYS:O	3:N:456:MET:HG2	2.11	0.50
1:B:80:LEU:HG	3:D:844:ALA:HA	1.94	0.50
3:D:1495:ILE:HD13	4:E:80:VAL:HG21	1.93	0.50
1:K:206:THR:HB	1:K:209:GLU:HG3	1.94	0.50
3:N:996:TRP:CD2	3:N:1056:PRO:HG3	2.46	0.50
2:C:614:ARG:NH2	2:C:618:GLY:O	2.44	0.50
2:C:797:GLY:O	2:C:829:GLN:NE2	2.45	0.50
2:M:413:LEU:HD21	2:M:451:LEU:HD13	1.92	0.50
3:D:903:ASP:OD1	10:D:2146:HOH:O	2.19	0.50
2:M:419:THR:H	2:M:422:ARG:HD3	1.76	0.50
5:P:380:GLU:CD	5:P:380:GLU:H	2.20	0.50
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.93	0.50
2:M:216:GLU:CD	2:M:216:GLU:H	2.18	0.50
2:M:627:ARG:NH2	2:M:640:ARG:HG3	2.27	0.50
3:N:1372:VAL:HA	3:N:1375:MET:HE3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:184:THR:O	1:A:192:LEU:HB2	2.12	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
5:P:410:TYR:O	5:P:414:ARG:CB	2.55	0.49
2:C:605:LYS:HB2	2:C:612:VAL:HB	1.94	0.49
2:C:1037:VAL:HG13	2:C:1049:LEU:HD11	1.94	0.49
5:F:163:LEU:HD13	5:F:174:LEU:HD13	1.95	0.49
5:P:89:GLY:C	5:P:90:GLN:NE2	2.70	0.49
3:D:171:LEU:HD22	3:D:390:PRO:HG2	1.94	0.49
5:F:270:LYS:HG2	5:F:295:MET:HE1	1.93	0.49
5:P:414:ARG:HD3	5:P:414:ARG:H	1.75	0.49
1:A:188:GLN:OE1	1:A:188:GLN:O	2.30	0.49
3:D:860:LEU:O	3:D:876:SER:HB2	2.13	0.49
3:D:1371:VAL:HG12	3:D:1375:MET:HE2	1.94	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
3:D:1100:ASP:OD1	3:D:1463:LYS:NZ	2.35	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:35:PRO:HG2	2:M:38:LYS:HD3	1.94	0.49
2:M:351:LEU:HD12	2:M:375:SER:HA	1.94	0.49
3:N:270:LEU:HD23	3:N:284:LEU:HD11	1.94	0.49
3:N:832:ARG:HD2	3:N:833:GLU:H	1.78	0.48
3:N:1208:ASP:HB2	3:N:1215:VAL:HG23	1.94	0.48
5:P:415:THR:HG21	5:P:416:ARG:NE	2.20	0.48
2:C:805:ARG:HG3	2:C:823:VAL:HG22	1.95	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:740:GLU:HB3	2:C:805:ARG:NH1	2.28	0.48
3:D:355:VAL:HG13	3:D:359:ALA:CB	2.43	0.48
1:L:216:GLU:OE1	1:L:219:ARG:NH2	2.36	0.48
1:A:188:GLN:HB3	1:A:189:ARG:HG2	1.96	0.48
3:D:832:ARG:HD2	3:D:833:GLU:H	1.78	0.48
3:D:248:PRO:HG3	3:D:308:LYS:HE3	1.96	0.48
3:D:1068:LEU:O	3:D:1072:ILE:HG12	2.13	0.48
5:F:372:ARG:HG2	5:F:386:VAL:HG21	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:GLU:OE1	1:B:219:ARG:NH2	2.36	0.48
3:D:1277:ILE:HG22	3:D:1278:ASP:H	1.78	0.48
2:M:682:TYR:CE1	3:N:635:PRO:HD2	2.48	0.48
3:N:1042:ARG:HB3	3:N:1057:VAL:HB	1.95	0.48
2:C:17:PRO:HB2	2:C:20:GLU:HB3	1.96	0.48
3:D:236:TYR:CD2	3:D:322:VAL:HG21	2.49	0.48
1:L:92:PRO:O	1:L:146:ARG:NH1	2.41	0.48
2:M:211:LEU:HD23	2:M:218:VAL:HG13	1.96	0.48
3:N:1281:VAL:HB	3:N:1317:ASP:H	1.78	0.48
3:N:1258:ARG:NH2	3:N:1351:GLU:HG2	2.28	0.48
2:C:194:VAL:HG22	2:C:221:LEU:HD23	1.95	0.48
3:D:808:THR:O	3:D:811:GLU:HB2	2.14	0.48
3:D:1310:ARG:HD2	3:D:1327:ARG:HD2	1.96	0.48
3:N:860:LEU:O	3:N:876:SER:HB2	2.13	0.48
5:P:354:LEU:O	5:P:358:LEU:HB2	2.14	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
2:M:577:PRO:HB3	2:M:993:PHE:CG	2.49	0.48
3:N:808:THR:O	3:N:811:GLU:HB2	2.14	0.48
3:D:999:THR:O	3:D:1003:VAL:HG13	2.14	0.47
1:L:56:VAL:HG22	1:L:142:VAL:HG12	1.96	0.47
1:B:80:LEU:HD11	3:D:842:VAL:HG12	1.96	0.47
1:K:107:LYS:HE3	1:K:107:LYS:HB2	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
3:D:959:GLU:HB3	3:D:963:TYR:CE1	2.48	0.47
1:K:27:PRO:HB2	1:K:192:LEU:HD13	1.96	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:C:774:LEU:HD23	5:F:354:LEU:HD21	1.96	0.47
1:L:108:GLU:HG2	1:L:131:THR:HG22	1.96	0.47
2:M:524:VAL:HG13	2:M:528:GLU:HB2	1.96	0.47
2:M:740:GLU:HB3	2:M:805:ARG:HH12	1.79	0.47
2:M:1058:ASP:OD1	3:N:621:LYS:HE2	2.14	0.47
2:C:409:ARG:HD2	2:C:452:ILE:HG22	1.95	0.47
2:C:680:ASP:OD1	3:D:943:THR:HG21	2.14	0.47
2:M:397:GLU:N	2:M:633:GLN:OE1	2.41	0.47
3:N:260:GLU:OE1	3:N:273:ARG:NH1	2.32	0.47
3:D:963:TYR:CE2	3:D:1002:LYS:HD3	2.49	0.47
3:D:1044:LEU:H	3:D:1044:LEU:HD12	1.78	0.47
3:D:1219:GLU:HG2	3:D:1221:VAL:HG23	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:GLU:OE1	1:A:139:ASN:ND2	2.44	0.47
1:B:56:VAL:HG22	1:B:142:VAL:HG12	1.97	0.47
2:C:168:ARG:HD3	2:C:268:ASP:CB	2.44	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
3:D:1236:LEU:HA	3:D:1359:GLN:HG3	1.96	0.47
2:M:195:LEU:O	2:M:199:VAL:HG23	2.14	0.47
2:M:722:ILE:HD12	2:M:821:GLU:HG3	1.97	0.47
2:M:911:GLU:O	2:M:915:LYS:HG2	2.15	0.47
2:M:966:LEU:HD13	2:M:986:PRO:HB3	1.96	0.47
3:N:82:LYS:HB2	3:N:84:ILE:HG22	1.95	0.47
1:A:70:GLY:HA3	1:A:136:GLY:HA2	1.97	0.47
2:C:524:VAL:HG13	2:C:528:GLU:HB2	1.96	0.47
2:C:1047:HIS:HE1	10:D:2160:HOH:O	1.97	0.47
2:M:679:PHE:HA	3:N:943:THR:HB	1.96	0.47
5:P:382:THR:OG1	5:P:385:GLU:OE2	2.33	0.47
5:F:80:PRO:HB2	5:F:210:LEU:HD11	1.96	0.47
1:K:70:GLY:N	2:M:607:ASP:OD1	2.47	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
3:N:47:GLU:CD	3:N:53:ILE:HG12	2.40	0.47
3:N:892:ASP:OD1	3:N:894:LYS:HD2	2.15	0.47
3:D:1168:MET:HE3	3:D:1171:VAL:HB	1.97	0.46
7:H:21:DA:H1'	7:H:22:DT:H5'	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
3:N:1342:GLU:CD	3:N:1342:GLU:H	2.23	0.46
5:P:193:ARG:HG2	7:R:7:DG:H5''	1.97	0.46
5:P:357:ALA:HB1	5:P:408:LEU:HD21	1.97	0.46
2:C:221:LEU:HD11	2:C:307:LEU:HD21	1.97	0.46
2:C:351:LEU:HD12	2:C:375:SER:HA	1.96	0.46
3:D:1168:MET:HE2	3:D:1172:HIS:CE1	2.50	0.46
3:D:1312:LEU:HD12	3:D:1324:PRO:HB2	1.97	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:911:GLU:O	2:C:915:LYS:HG2	2.16	0.46
2:M:587:VAL:O	2:M:591:SER:OG	2.30	0.46
3:N:71:LYS:O	3:N:80:VAL:HG22	2.15	0.46
3:N:1364:HIS:ND1	3:N:1366:LYS:HB2	2.30	0.46
1:A:227:ASN:HA	1:A:228:PRO:HD3	1.75	0.46
2:C:598:GLU:O	2:C:651:LYS:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:504:GLU:HG2	2:M:509:ALA:HB2	1.98	0.46
2:M:772:ARG:HE	5:P:373:LYS:HD2	1.80	0.46
3:N:438:ASP:OD1	3:N:441:ARG:NH2	2.49	0.46
1:B:108:GLU:HG2	1:B:131:THR:HG22	1.97	0.46
2:C:134:ARG:NH1	2:C:392:SER:O	2.49	0.46
3:D:527:MET:HB2	3:D:527:MET:HE2	1.80	0.46
2:M:797:GLY:O	2:M:829:GLN:NE2	2.48	0.46
3:N:1047:LYS:HG2	3:N:1053:PHE:CZ	2.50	0.46
2:C:1057:SER:HB3	2:C:1058:ASP:H	1.51	0.46
3:D:892:ASP:OD1	3:D:894:LYS:HD2	2.15	0.46
2:M:580:MET:HB3	2:M:584:GLU:CD	2.41	0.46
2:M:711:GLU:HG2	2:M:822:VAL:HG22	1.97	0.46
2:M:872:ASN:ND2	3:N:784:ASP:OD1	2.39	0.46
3:N:954:ALA:HB3	3:N:1062:ARG:HG3	1.97	0.46
2:C:64:LEU:HD22	2:C:100:LEU:HD11	1.97	0.46
2:C:163:ILE:HG23	2:C:171:TRP:CE2	2.51	0.46
2:C:722:ILE:HD12	2:C:821:GLU:HG3	1.97	0.46
2:C:881:ASN:OD1	2:C:881:ASN:N	2.49	0.46
5:F:201:LYS:NZ	5:F:244:ARG:HH22	2.14	0.46
1:A:39:PRO:HG3	1:B:39:PRO:HG3	1.98	0.46
1:B:80:LEU:HB3	3:D:867:ARG:NH2	2.31	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
2:C:504:GLU:HG2	2:C:509:ALA:HB2	1.98	0.46
3:D:236:TYR:CZ	3:D:242:LEU:HD12	2.51	0.46
5:F:162:LYS:HB2	5:F:162:LYS:HE3	1.72	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
3:N:44:LEU:HB3	3:N:525:ARG:NH2	2.30	0.46
3:N:586:ARG:HH22	6:Q:10:DG:H5''	1.80	0.46
3:D:34:TYR:CZ	3:D:35:ARG:HG3	2.51	0.46
1:K:188:GLN:HG3	1:K:189:ARG:HG3	1.98	0.46
1:L:124:ASN:OD1	1:L:124:ASN:N	2.49	0.45
2:M:69:LEU:HD12	2:M:97:ARG:HG2	1.98	0.45
5:P:77:THR:O	5:P:78:SER:CB	2.64	0.45
3:D:1189:ARG:HB3	3:D:1204:CYS:HA	1.98	0.45
4:E:68:LEU:HD12	4:E:68:LEU:HA	1.77	0.45
3:N:741:ASP:OD1	3:N:743:ASP:OD1	2.34	0.45
7:R:21:DA:H5'	7:R:21:DA:C8	2.51	0.45
7:R:21:DA:H5'	7:R:21:DA:H8	1.82	0.45
1:A:57:TYR:CG	1:A:161:ARG:HD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:331:ARG:NH2	10:C:1304:HOH:O	2.49	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
2:C:172:ILE:CG1	2:C:186:VAL:HG22	2.47	0.45
5:F:333:ILE:HA	5:F:334:PRO:HD3	1.79	0.45
1:L:176:ARG:NH2	3:N:888:GLU:OE1	2.49	0.45
2:M:397:GLU:HG3	2:M:631:SER:HB2	1.98	0.45
1:A:188:GLN:OE1	1:A:188:GLN:C	2.60	0.45
2:C:157:ARG:HA	2:C:157:ARG:HD3	1.77	0.45
3:D:405:ASP:CG	3:D:406:ASP:H	2.25	0.45
2:M:328:LEU:HA	2:M:328:LEU:HD23	1.82	0.45
2:M:436:GLY:HA2	2:M:538:GLN:O	2.15	0.45
2:C:966:LEU:HD13	2:C:986:PRO:HB3	1.97	0.45
3:D:957:PRO:HG3	3:D:1007:VAL:HA	1.99	0.45
1:L:78:ILE:HG21	1:L:140:MET:HE1	1.99	0.45
2:M:1090:LYS:NZ	10:M:1230:HOH:O	2.50	0.45
1:K:57:TYR:CG	1:K:161:ARG:HD2	2.51	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
3:D:704:ARG:HB2	3:D:745:MET:HE2	1.98	0.45
2:M:187:ASN:HD22	2:M:187:ASN:HA	1.60	0.45
2:M:251:ASP:OD1	2:M:251:ASP:N	2.47	0.45
2:M:1102:LEU:HB2	3:N:7:LYS:HB2	1.99	0.45
5:P:415:THR:HG21	5:P:416:ARG:CZ	2.46	0.45
2:C:168:ARG:HD3	2:C:268:ASP:HB3	1.99	0.45
3:D:230:TRP:CZ2	3:D:232:GLU:HG2	2.51	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
2:M:948:GLU:HB3	2:M:953:VAL:HG23	1.98	0.45
3:N:405:ASP:CG	3:N:406:ASP:H	2.25	0.45
1:A:112:ARG:HD2	10:A:412:HOH:O	2.17	0.45
2:C:247:PRO:HA	2:C:248:PRO:HD3	1.65	0.45
5:F:400:ILE:HA	5:F:403:LYS:HG2	1.98	0.45
2:M:67:ASP:OD1	2:M:68:PHE:N	2.50	0.45
2:M:249:LYS:NZ	2:M:251:ASP:OD1	2.49	0.45
3:N:1495:ILE:HD13	4:O:80:VAL:HG21	1.98	0.45
1:B:34:VAL:HG12	1:B:181:VAL:HG21	1.99	0.44
1:B:58:ILE:HG12	1:B:140:MET:HE2	1.99	0.44
2:C:740:GLU:HB3	2:C:805:ARG:HH12	1.81	0.44
3:D:131:LYS:O	3:D:456:MET:HG2	2.16	0.44
2:M:172:ILE:HG12	2:M:186:VAL:CG2	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:59:ALA:HB2	3:N:78:VAL:HG21	1.99	0.44
3:N:489:ARG:NH1	3:N:1391:GLU:OE2	2.50	0.44
3:N:1461:GLY:O	3:N:1465:ASN:ND2	2.49	0.44
5:P:364:ARG:HH12	5:P:392:VAL:HG11	1.82	0.44
1:B:91:ASN:HB3	1:B:94:LEU:HB2	1.99	0.44
1:B:124:ASN:OD1	1:B:124:ASN:N	2.51	0.44
2:C:6:PHE:CD2	2:C:909:ALA:HB2	2.52	0.44
2:C:12:VAL:HG21	2:C:472:ARG:HD3	1.99	0.44
2:C:874:LEU:HD23	3:D:1023:MET:SD	2.57	0.44
3:D:134:VAL:HG22	3:D:151:GLN:H	1.82	0.44
1:L:58:ILE:HG12	1:L:140:MET:HE2	1.99	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
5:P:329:TYR:CE2	5:P:333:ILE:HD11	2.53	0.44
1:B:64:GLU:HA	1:B:165:ILE:HD13	2.00	0.44
7:H:3:DT:H2'	7:H:4:DA:C8	2.52	0.44
1:K:115:LEU:HA	1:K:116:PRO:HD3	1.82	0.44
2:M:404:LEU:O	2:M:408:ARG:HG3	2.16	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
2:C:1001:VAL:HG13	3:D:630:VAL:HB	1.99	0.44
3:D:959:GLU:OE1	3:D:959:GLU:N	2.50	0.44
3:N:801:GLY:O	3:N:804:LEU:HG	2.18	0.44
2:C:203:ASP:OD2	2:C:204:GLN:N	2.51	0.44
2:C:356:ARG:HA	2:C:359:MET:HE2	1.99	0.44
2:C:976:ASP:OD1	2:C:978:ARG:HD3	2.17	0.44
3:D:939:PHE:O	3:D:943:THR:HG22	2.18	0.44
1:K:59:GLU:OE1	1:K:139:ASN:ND2	2.44	0.44
2:M:1054:THR:O	2:M:1059:ASP:HB3	2.18	0.44
3:N:527:MET:HE2	3:N:527:MET:HB2	1.84	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
3:N:1232:PRO:HG2	3:N:1356:TYR:HE2	1.82	0.44
1:A:206:THR:HG22	1:A:208:LEU:H	1.83	0.44
1:B:78:ILE:HG21	1:B:140:MET:HE1	1.99	0.44
2:M:858:MET:HG2	2:M:867:VAL:O	2.18	0.44
3:N:689:ASP:O	3:N:693:GLU:HG3	2.18	0.44
5:P:188:ILE:HD13	5:P:221:ILE:HG12	1.98	0.44
5:P:403:LYS:HA	5:P:406:ARG:HG2	1.98	0.44
2:C:328:LEU:HA	2:C:328:LEU:HD23	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:134:VAL:HG23	3:D:149:LYS:HA	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:M:395:LYS:HE2	2:M:403:SER:HB3	2.00	0.44
3:N:134:VAL:HG22	3:N:151:GLN:H	1.82	0.44
1:A:8:ALA:HA	1:A:9:PRO:HD3	1.66	0.44
3:D:223:LEU:HD11	3:D:288:MET:HE1	1.99	0.44
3:D:438:ASP:OD1	3:D:441:ARG:NH2	2.49	0.44
5:F:370:LYS:HB3	5:F:376:ILE:HG13	2.00	0.44
2:M:224:GLU:CD	2:M:224:GLU:H	2.25	0.44
3:N:939:PHE:O	3:N:943:THR:HG22	2.18	0.44
2:C:577:PRO:HB3	2:C:993:PHE:CG	2.53	0.43
2:M:28:ARG:HH12	2:M:42:VAL:HG11	1.83	0.43
2:M:356:ARG:HA	2:M:359:MET:HE2	1.99	0.43
3:N:536:ALA:HA	5:P:315:VAL:O	2.18	0.43
5:P:77:THR:O	5:P:77:THR:HG23	2.18	0.43
2:C:172:ILE:HG13	2:C:186:VAL:HG22	2.00	0.43
3:D:1042:ARG:HB3	3:D:1057:VAL:HB	2.00	0.43
4:E:45:ARG:HA	4:E:46:PRO:HD3	1.92	0.43
5:F:392:VAL:HB	5:F:396:ARG:HG2	1.99	0.43
1:L:80:LEU:HD11	3:N:842:VAL:HG12	2.00	0.43
2:M:764:GLU:HG2	3:N:54:LYS:NZ	2.33	0.43
2:M:930:LYS:HE3	2:M:935:GLY:HA2	2.01	0.43
1:B:49:PRO:HA	1:B:148:VAL:HG12	1.99	0.43
5:F:319:THR:HA	5:F:320:PRO:HD3	1.86	0.43
2:M:150:PRO:HG3	2:M:322:VAL:HG11	2.00	0.43
3:N:44:LEU:HB3	3:N:525:ARG:HH21	1.83	0.43
3:N:46:ASP:HB3	3:N:49:ILE:HD12	2.01	0.43
3:N:134:VAL:HG23	3:N:149:LYS:HA	2.01	0.43
3:N:1018:ASN:HA	3:N:1019:PRO:HD3	1.92	0.43
1:A:9:PRO:HG3	10:A:407:HOH:O	2.18	0.43
2:C:230:ARG:HG3	2:C:233:GLU:HG3	2.00	0.43
2:C:404:LEU:O	2:C:408:ARG:HG3	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:M:876:VAL:HB	3:N:949:ILE:HD12	2.00	0.43
2:C:954:THR:HA	2:C:955:PRO:HD3	1.88	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
1:K:6:LEU:HD11	1:K:27:PRO:HG2	1.99	0.43
2:M:409:ARG:HH11	2:M:409:ARG:CG	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:874:LEU:HD23	3:N:1023:MET:SD	2.58	0.43
2:M:1053:LEU:HA	3:N:621:LYS:HD2	2.01	0.43
3:N:704:ARG:HB2	3:N:745:MET:HE2	1.99	0.43
3:N:1459:LEU:HD12	3:N:1464:GLU:HB3	1.99	0.43
5:P:333:ILE:HA	5:P:334:PRO:HD3	1.87	0.43
5:P:412:GLU:HA	5:P:416:ARG:HE	1.81	0.43
1:A:107:LYS:HE3	1:A:107:LYS:HB2	1.71	0.43
3:D:1031:ASN:O	3:D:1035:ILE:HG12	2.19	0.43
3:N:371:ILE:HD12	5:P:230:LYS:HA	2.01	0.43
3:N:711:LEU:HD13	3:N:778:LEU:HD13	2.00	0.43
5:P:371:LEU:HD22	5:P:381:HIS:CE1	2.53	0.43
2:C:97:ARG:NH1	2:C:110:GLU:OE1	2.51	0.43
3:D:44:LEU:HB3	3:D:525:ARG:HH21	1.83	0.43
3:D:1147:ARG:HD3	3:D:1188:VAL:HG11	2.01	0.43
1:K:36:LEU:HD23	1:K:36:LEU:HA	1.80	0.43
2:M:728:HIS:CD2	5:P:422:LEU:HD13	2.53	0.43
2:M:1051:GLU:HB3	2:M:1056:LYS:HD2	2.00	0.43
5:P:397:ILE:HA	5:P:400:ILE:HG22	2.01	0.43
2:C:948:GLU:HB3	2:C:953:VAL:HG23	1.99	0.43
3:D:17:LYS:HB2	3:D:17:LYS:HE3	1.70	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
5:P:155:THR:O	5:P:159:ILE:HG12	2.19	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
2:M:154:ARG:NH2	2:M:157:ARG:HG3	2.33	0.43
2:M:211:LEU:HD21	2:M:311:PHE:CE2	2.54	0.43
2:M:627:ARG:HD2	2:M:627:ARG:HA	1.53	0.43
2:M:1102:LEU:HD23	2:M:1108:PRO:HA	2.01	0.43
3:N:1107:VAL:HA	3:N:1200:VAL:O	2.19	0.43
5:P:410:TYR:O	5:P:414:ARG:HG2	2.18	0.43
1:B:44:LEU:HD13	1:B:199:ILE:HD13	2.00	0.43
1:B:211:LEU:O	1:B:215:VAL:HG22	2.19	0.43
2:C:771:GLU:O	2:C:775:ARG:HB2	2.19	0.43
2:C:774:LEU:HD22	2:C:774:LEU:HA	1.82	0.43
3:D:536:ALA:HA	5:F:315:VAL:O	2.19	0.43
3:D:1258:ARG:HH21	3:D:1351:GLU:CG	2.32	0.43
3:N:483:HIS:HA	3:N:484:PRO:HD3	1.91	0.43
3:N:589:ALA:HA	3:N:590:PRO:HD3	1.91	0.43
3:N:1478:SER:O	3:N:1482:ARG:HB2	2.19	0.43
1:A:6:LEU:HD13	1:A:7:LYS:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1102:LEU:HD23	2:C:1108:PRO:HA	2.01	0.42
5:F:338:LEU:HD23	5:F:339:PRO:HD2	2.01	0.42
2:M:35:PRO:HA	2:M:36:PRO:HD3	1.95	0.42
2:M:184:MET:HE2	2:M:191:PHE:CZ	2.54	0.42
2:M:535:SER:O	2:M:538:GLN:HG2	2.18	0.42
2:M:684:PHE:HE1	3:N:783:ARG:HB2	1.84	0.42
3:N:1258:ARG:HH21	3:N:1351:GLU:CG	2.31	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:96:ALA:HB3	3:N:554:LEU:HD23	2.00	0.42
3:N:434:ARG:NH2	5:P:135:ILE:O	2.52	0.42
3:N:879:ARG:HD3	3:N:902:LEU:O	2.19	0.42
3:D:684:LYS:HE2	3:D:684:LYS:HB3	1.85	0.42
5:F:188:ILE:HG12	5:F:224:VAL:HG21	2.01	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
5:P:329:TYR:HE2	5:P:333:ILE:HD11	1.84	0.42
2:C:144:PRO:HG2	2:C:165:LEU:HD23	2.01	0.42
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
3:D:1258:ARG:NH2	3:D:1351:GLU:HG2	2.35	0.42
5:F:372:ARG:HD3	5:F:401:GLU:OE2	2.20	0.42
2:M:348:LEU:HD12	2:M:348:LEU:HA	1.92	0.42
4:O:17:TYR:O	4:O:21:VAL:HG23	2.20	0.42
7:R:18:DC:H2"	7:R:19:DG:C8	2.54	0.42
1:A:36:LEU:HA	1:A:36:LEU:HD23	1.79	0.42
1:B:111:ALA:HB3	1:B:125:PRO:C	2.44	0.42
10:C:1268:HOH:O	5:F:280:GLN:HG2	2.18	0.42
3:D:42:ASP:OD1	3:D:48:ARG:NH2	2.53	0.42
2:M:35:PRO:HG2	2:M:38:LYS:HB2	2.02	0.42
2:M:77:PRO:HB2	2:M:78:PHE:CD1	2.53	0.42
2:M:976:ASP:OD1	2:M:978:ARG:HD3	2.18	0.42
3:N:897:TRP:HH2	3:N:902:LEU:HD22	1.84	0.42
1:A:180:GLN:NE2	2:C:935:GLY:O	2.52	0.42
2:C:792:VAL:HA	2:C:793:PRO:HD3	1.89	0.42
1:K:206:THR:HG22	1:K:208:LEU:H	1.84	0.42
2:M:239:PHE:CD2	2:M:253:ALA:HA	2.53	0.42
3:N:1373:ARG:HD3	10:N:2143:HOH:O	2.19	0.42
1:K:201:THR:HG21	1:K:205:VAL:O	2.20	0.42
2:M:230:ARG:HB2	2:M:231:PRO:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1304:LYS:HE2	3:N:1304:LYS:HB3	1.86	0.42
3:D:1144:LEU:HD23	3:D:1144:LEU:HA	1.79	0.42
2:C:179:ASN:OD1	2:C:181:VAL:HG12	2.20	0.42
2:C:229:MET:HB2	2:C:233:GLU:HB2	2.01	0.42
2:C:944:LEU:HD23	2:C:944:LEU:HA	1.92	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
1:L:156:HIS:ND1	1:L:158:ILE:HG12	2.34	0.42
2:M:592:LEU:HD23	2:M:592:LEU:HA	1.80	0.42
2:C:269:LEU:HB2	2:C:288:ARG:O	2.20	0.42
5:F:88:ILE:HA	5:F:88:ILE:HD12	1.75	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
3:N:1071:PHE:O	3:N:1074:SER:OG	2.29	0.42
3:N:1208:ASP:OD1	3:N:1210:SER:OG	2.33	0.42
3:N:1284:GLU:HB3	3:N:1291:SER:HB3	2.01	0.42
3:N:1353:GLN:HG2	3:N:1368:ILE:HD12	2.01	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
1:A:11:PHE:O	1:B:228:PRO:HA	2.20	0.41
2:C:858:MET:HG2	2:C:867:VAL:O	2.20	0.41
2:C:1102:LEU:HB2	3:D:7:LYS:HB2	2.02	0.41
4:E:40:LEU:HG	4:E:67:GLU:HG2	2.01	0.41
1:K:6:LEU:HD13	1:K:7:LYS:H	1.85	0.41
3:N:707:THR:HG23	3:N:712:GLY:HA3	2.01	0.41
1:B:156:HIS:ND1	1:B:158:ILE:HG12	2.35	0.41
3:D:275:GLU:HB3	3:D:276:ASP:H	1.69	0.41
3:D:355:VAL:HG13	3:D:359:ALA:HB3	2.01	0.41
3:D:1348:LEU:HD23	3:D:1348:LEU:HA	1.92	0.41
4:E:3:GLU:HA	4:E:4:PRO:HD3	1.93	0.41
2:M:657:ASP:OD2	2:M:663:ASN:N	2.48	0.41
3:N:842:VAL:HG22	3:N:865:THR:HB	2.02	0.41
5:P:83:GLN:O	5:P:87:GLU:HG3	2.20	0.41
7:R:15:DT:H2''	7:R:16:DC:H5'	2.02	0.41
2:C:224:GLU:H	2:C:224:GLU:CD	2.26	0.41
2:C:535:SER:O	2:C:538:GLN:HG2	2.20	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
4:O:89:MET:HE3	4:O:93:TYR:HE1	1.86	0.41
5:P:319:THR:HA	5:P:320:PRO:HD3	1.92	0.41
2:C:89:THR:O	2:C:91:GLN:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:F:273:ARG:NH1	10:F:2108:HOH:O	2.54	0.41
5:F:397:ILE:HA	5:F:400:ILE:HG12	2.02	0.41
1:L:175:ARG:N	1:L:200:TRP:O	2.50	0.41
3:N:90:MET:HE2	3:N:90:MET:HB3	1.94	0.41
3:N:521:PRO:HA	3:N:522:PRO:HD3	1.91	0.41
3:D:842:VAL:HG22	3:D:865:THR:HB	2.02	0.41
4:E:36:LYS:HB3	4:E:36:LYS:HE3	1.81	0.41
2:M:591:SER:O	2:M:592:LEU:CB	2.55	0.41
2:M:786:LYS:HE2	2:M:786:LYS:HB3	1.81	0.41
3:N:493:ARG:NH1	10:N:2150:HOH:O	2.48	0.41
5:P:80:PRO:HB2	5:P:210:LEU:HD11	2.02	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:H	3:N:486:ARG:HG3	1.52	0.41
4:O:14:ASP:OD2	4:O:14:ASP:N	2.54	0.41
4:O:83:ASP:OD1	4:O:83:ASP:N	2.53	0.41
1:A:201:THR:HG21	1:A:205:VAL:O	2.20	0.41
3:D:237:LYS:N	3:D:240:GLU:OE1	2.46	0.41
1:K:11:PHE:O	1:L:228:PRO:HA	2.21	0.41
2:M:942:GLU:HG2	2:M:945:ARG:HH21	1.85	0.41
3:N:206:ARG:HA	3:N:206:ARG:HD2	1.77	0.41
5:P:399:GLN:HG3	5:P:403:LYS:HE2	2.02	0.41
1:B:220:GLU:O	1:B:223:THR:OG1	2.31	0.41
2:C:462:ASP:OD2	2:C:468:ARG:NH1	2.51	0.41
3:D:41:ARG:HG3	3:D:48:ARG:HE	1.85	0.41
3:D:586:ARG:HH22	6:G:10:DG:H5"	1.86	0.41
4:E:14:ASP:OD2	4:E:14:ASP:N	2.54	0.41
5:F:140:ARG:HE	5:F:140:ARG:HB2	1.60	0.41
10:F:2110:HOH:O	7:H:1:DT:H72	2.21	0.41
1:K:41:ARG:HA	1:K:177:VAL:HG11	2.03	0.41
3:N:103:TRP:HB3	3:N:1448:THR:CG2	2.51	0.41
3:N:465:LEU:HD12	3:N:513:ILE:HD13	2.01	0.41
5:P:360:LYS:HZ2	5:P:416:ARG:HH22	1.66	0.41
5:P:422:LEU:HD23	5:P:422:LEU:HA	1.89	0.41
1:B:115:LEU:HA	1:B:116:PRO:HD3	1.91	0.41
2:C:160:ALA:HB3	2:C:174:LEU:HB2	2.02	0.41
2:C:200:LEU:HD13	2:C:300:ASP:HB2	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:939:ARG:H	2:C:939:ARG:HG2	1.67	0.41
2:C:1038:TRP:CE2	3:D:1099:VAL:HG11	2.56	0.41
2:C:1043:TYR:CD1	3:D:763:MET:HG2	2.55	0.41
3:D:618:LEU:HG	3:D:1467:ILE:HG23	2.03	0.41
3:D:879:ARG:HD3	3:D:902:LEU:O	2.21	0.41
3:D:1000:THR:HG23	3:D:1036:ARG:HD2	2.03	0.41
1:K:31:GLY:N	1:K:193:ASP:OD1	2.47	0.41
1:K:100:LEU:HD23	1:K:141:GLU:HG2	2.03	0.41
2:M:12:VAL:HG21	2:M:472:ARG:HD3	2.03	0.41
2:M:136:ILE:HD13	2:M:392:SER:HA	2.03	0.41
2:M:464:LEU:HD12	2:M:464:LEU:HA	1.84	0.41
2:M:944:LEU:HD23	2:M:944:LEU:HA	1.91	0.41
3:N:50:PHE:CD2	3:N:522:PRO:HD3	2.56	0.41
3:N:84:ILE:O	3:N:87:ARG:HG3	2.21	0.41
4:O:57:ASP:HA	4:O:58:PRO:HD3	1.89	0.41
2:C:107:LEU:HD22	2:C:108:ILE:N	2.36	0.41
3:D:428:LYS:HE2	3:D:428:LYS:HB3	1.93	0.41
3:D:1057:VAL:HG13	3:D:1069:GLU:CD	2.46	0.41
3:D:1217:ILE:HD12	3:D:1480:PHE:CZ	2.56	0.41
3:D:1387:SER:HB3	3:D:1407:LEU:HD11	2.03	0.41
3:D:1463:LYS:HE2	3:D:1463:LYS:HB3	1.90	0.41
5:F:79:ASP:HA	5:F:80:PRO:HD3	1.91	0.41
2:M:91:GLN:HB2	2:M:117:HIS:HB3	2.02	0.41
2:M:232:GLU:HG2	2:M:250:ARG:HD2	2.02	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
4:O:46:PRO:HD2	4:O:63:TRP:CE2	2.56	0.41
2:C:236:ILE:O	2:C:240:THR:HG23	2.20	0.40
2:C:642:ARG:HA	2:C:642:ARG:HD3	1.84	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
1:L:91:ASN:HB3	1:L:94:LEU:HB2	2.02	0.40
2:M:561:GLY:O	2:M:565:GLN:HG3	2.21	0.40
3:N:288:MET:HE2	3:N:307:ALA:HB2	2.02	0.40
3:N:684:LYS:HB3	3:N:684:LYS:HE2	1.85	0.40
2:C:942:GLU:HG2	2:C:945:ARG:HH21	1.85	0.40
3:D:314:PRO:HB2	3:D:317:VAL:HG12	2.03	0.40
3:D:1205:TYR:CZ	3:D:1366:LYS:HD3	2.56	0.40
2:M:232:GLU:CG	2:M:250:ARG:HD2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:593:ALA:HB1	2:M:659:PRO:HD2	2.03	0.40
3:N:219:GLU:HB2	3:N:339:TRP:HH2	1.86	0.40
3:N:468:LEU:HD23	3:N:468:LEU:HA	1.92	0.40
3:N:731:LEU:HD23	3:N:731:LEU:HA	1.92	0.40
3:N:1010:ASN:OD1	3:N:1014:ASN:ND2	2.47	0.40
3:N:1383:ASP:HA	3:N:1384:PRO:HD3	1.84	0.40
3:D:114:THR:HG23	3:D:495:ARG:HG2	2.03	0.40
3:D:462:GLN:HB2	3:D:513:ILE:HG21	2.02	0.40
2:M:881:ASN:OD1	2:M:881:ASN:N	2.50	0.40
5:P:140:ARG:CG	5:P:142:ARG:HH22	2.27	0.40
5:P:256:ARG:NH2	5:P:311:ALA:O	2.54	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:F:364:ARG:HG2	5:F:390:PHE:CE2	2.57	0.40
1:K:32:PHE:HA	1:K:35:THR:HB	2.03	0.40
2:M:135:VAL:HG23	2:M:395:LYS:HG3	2.03	0.40
3:N:834:THR:OG1	3:N:838:ARG:HD2	2.21	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
5:P:365:GLU:HA	5:P:368:VAL:HG22	2.03	0.40
1:A:111:ALA:HB3	1:A:125:PRO:HA	2.04	0.40
3:D:475:LYS:O	3:D:479:GLU:HG2	2.22	0.40
3:D:890:VAL:HB	3:D:922:LEU:HD13	2.04	0.40
4:E:83:ASP:OD1	4:E:83:ASP:N	2.54	0.40
1:K:65:PHE:O	2:M:628:PHE:CE2	2.75	0.40
2:M:571:LEU:HD22	2:M:700:TYR:HA	2.02	0.40
2:M:1057:SER:HB3	2:M:1058:ASP:H	1.55	0.40
3:N:45:PHE:O	3:N:86:ARG:NH2	2.54	0.40
3:N:215:TYR:HE1	3:N:381:ALA:H	1.70	0.40
3:N:284:LEU:HA	3:N:285:PRO:HD2	1.94	0.40
3:N:487:ALA:O	3:N:491:LYS:HG2	2.21	0.40
3:N:890:VAL:HB	3:N:922:LEU:HD13	2.04	0.40
3:N:952:ASP:HA	3:N:1062:ARG:NH2	2.36	0.40
3:N:1468:LEU:HB3	3:N:1470:ARG:HG3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	224/315 (71%)	222 (99%)	2 (1%)	0	100	100
1	B	220/315 (70%)	215 (98%)	5 (2%)	0	100	100
1	K	10/315 (3%)	10 (100%)	0	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%)	48	77
3	N	1482/1524 (97%)	1454 (98%)	27 (2%)	1 (0%)	48	77
4	E	92/99 (93%)	89 (97%)	2 (2%)	1 (1%)	11	36
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	6728/7630 (88%)	6599 (98%)	126 (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

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%)	183 (92%)	16 (8%)	11	34
1	B	195/273 (71%)	181 (93%)	14 (7%)	13	39
1	K	199/273 (73%)	186 (94%)	13 (6%)	15	44
1	L	198/273 (72%)	186 (94%)	12 (6%)	17	46
2	C	936/941 (100%)	858 (92%)	78 (8%)	10	32
2	M	936/941 (100%)	864 (92%)	72 (8%)	12	35
3	D	1253/1279 (98%)	1152 (92%)	101 (8%)	11	33
3	N	1253/1279 (98%)	1153 (92%)	100 (8%)	11	34
4	E	83/88 (94%)	82 (99%)	1 (1%)	63	86
4	O	83/88 (94%)	81 (98%)	2 (2%)	43	75
5	F	301/388 (78%)	285 (95%)	16 (5%)	20	52
5	P	302/388 (78%)	264 (87%)	38 (13%)	4	14
All	All	5938/6484 (92%)	5475 (92%)	463 (8%)	11	35

All (463) 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	112	ARG
1	A	126	ASP
1	A	142	VAL
1	A	148	VAL
1	A	184	THR
1	A	186	LEU
1	A	188	GLN
1	A	189	ARG
1	A	205	VAL
1	A	206	THR
1	A	219	ARG
1	A	229	GLN
1	B	34	VAL
1	B	56	VAL
1	B	80	LEU
1	B	94	LEU
1	B	112	ARG
1	B	133	GLU

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Mol	Chain	Res	Type
1	B	142	VAL
1	B	158	ILE
1	B	186	LEU
1	B	189	ARG
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	172	ILE
2	C	177	GLU
2	C	182	VAL
2	C	194	VAL
2	C	196	LEU
2	C	205	GLU
2	C	218	VAL
2	C	221	LEU
2	C	232	GLU
2	C	251	ASP
2	C	261	ILE
2	C	265	ARG
2	C	322	VAL
2	C	331	ARG
2	C	336	VAL
2	C	342	ASP
2	C	358	ARG
2	C	372	LEU
2	C	395	LYS
2	C	403	SER
2	C	418	LEU
2	C	427	VAL
2	C	454	SER
2	C	464	LEU
2	C	480	THR

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Mol	Chain	Res	Type
2	C	482	GLU
2	C	511	GLU
2	C	512	ARG
2	C	513	VAL
2	C	524	VAL
2	C	575	GLN
2	C	578	VAL
2	C	583	LEU
2	C	584	GLU
2	C	586	ARG
2	C	589	ARG
2	C	591	SER
2	C	592	LEU
2	C	617	ASP
2	C	633	GLN
2	C	638	ASP
2	C	640	ARG
2	C	648	ARG
2	C	670	GLN
2	C	683	ASN
2	C	715	THR
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	820	ARG
2	C	830	LYS
2	C	848	VAL
2	C	905	ILE
2	C	910	LYS
2	C	916	GLU
2	C	923	GLU
2	C	928	LYS
2	C	939	ARG
2	C	952	LEU
2	C	968	LEU
2	C	978	ARG
2	C	1001	VAL
2	C	1014	SER

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Mol	Chain	Res	Type
2	C	1057	SER
2	C	1080	SER
3	D	30	GLU
3	D	64	LYS
3	D	81	THR
3	D	106	LYS
3	D	135	LEU
3	D	141	ILE
3	D	142	LEU
3	D	155	ASP
3	D	161	LEU
3	D	179	VAL
3	D	186	VAL
3	D	190	GLU
3	D	191	LEU
3	D	198	ARG
3	D	204	LEU
3	D	230	TRP
3	D	231	VAL
3	D	234	GLU
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	355	VAL
3	D	360	ARG
3	D	362	GLU
3	D	372	ASP
3	D	387	LEU
3	D	411	THR
3	D	415	VAL
3	D	421	LEU
3	D	427	VAL
3	D	500	ARG
3	D	525	ARG
3	D	548	ILE
3	D	572	ARG
3	D	576	GLU

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Mol	Chain	Res	Type
3	D	586	ARG
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	675	ARG
3	D	686	GLU
3	D	709	HIS
3	D	754	PHE
3	D	778	LEU
3	D	808	THR
3	D	810	GLU
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	907	GLU
3	D	908	LYS
3	D	943	THR
3	D	972	LEU
3	D	983	LEU
3	D	984	THR
3	D	995	LEU
3	D	1041	LEU
3	D	1055	VAL
3	D	1062	ARG
3	D	1067	VAL
3	D	1079	LYS
3	D	1127	GLU
3	D	1128	VAL
3	D	1152	GLU
3	D	1155	VAL
3	D	1162	GLU
3	D	1188	VAL
3	D	1195	GLN

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Mol	Chain	Res	Type
3	D	1208	ASP
3	D	1219	GLU
3	D	1221	VAL
3	D	1234	THR
3	D	1277	ILE
3	D	1283	ILE
3	D	1284	GLU
3	D	1287	GLU
3	D	1290	LEU
3	D	1304	LYS
3	D	1305	LEU
3	D	1313	VAL
3	D	1317	ASP
3	D	1455	LYS
3	D	1470	ARG
3	D	1486	VAL
3	D	1493	LYS
3	D	1496	GLU
3	D	1501	GLU
4	E	50	THR
5	F	88	ILE
5	F	122	LEU
5	F	123	ASP
5	F	141	VAL
5	F	150	THR
5	F	172	ARG
5	F	205	ARG
5	F	208	SER
5	F	218	GLN
5	F	279	GLN
5	F	295	MET
5	F	310	ILE
5	F	364	ARG
5	F	377	ASP
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

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Mol	Chain	Res	Type
1	K	148	VAL
1	K	184	THR
1	K	186	LEU
1	K	205	VAL
1	K	206	THR
1	K	219	ARG
1	K	229	GLN
1	L	34	VAL
1	L	56	VAL
1	L	62	LEU
1	L	80	LEU
1	L	142	VAL
1	L	158	ILE
1	L	186	LEU
1	L	189	ARG
1	L	197	LEU
1	L	199	ILE
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	154	ARG
2	M	157	ARG
2	M	172	ILE
2	M	174	LEU
2	M	177	GLU
2	M	182	VAL
2	M	187	ASN
2	M	194	VAL
2	M	196	LEU
2	M	216	GLU
2	M	217	LEU
2	M	224	GLU
2	M	250	ARG
2	M	251	ASP
2	M	252	LYS
2	M	261	ILE
2	M	265	ARG

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Mol	Chain	Res	Type
2	M	322	VAL
2	M	331	ARG
2	M	336	VAL
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	454	SER
2	M	464	LEU
2	M	480	THR
2	M	482	GLU
2	M	511	GLU
2	M	512	ARG
2	M	513	VAL
2	M	524	VAL
2	M	575	GLN
2	M	578	VAL
2	M	583	LEU
2	M	584	GLU
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	715	THR
2	M	768	THR
2	M	813	VAL
2	M	815	LEU
2	M	820	ARG
2	M	830	LYS
2	M	848	VAL
2	M	905	ILE
2	M	910	LYS
2	M	916	GLU
2	M	923	GLU
2	M	928	LYS

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Mol	Chain	Res	Type
2	M	939	ARG
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	106	LYS
3	N	135	LEU
3	N	141	ILE
3	N	142	LEU
3	N	155	ASP
3	N	161	LEU
3	N	179	VAL
3	N	186	VAL
3	N	190	GLU
3	N	191	LEU
3	N	198	ARG
3	N	204	LEU
3	N	211	VAL
3	N	225	LEU
3	N	227	LEU
3	N	231	VAL
3	N	256	GLU
3	N	270	LEU
3	N	277	GLU
3	N	286	VAL
3	N	293	VAL
3	N	306	GLU
3	N	311	LEU
3	N	316	GLN
3	N	322	VAL
3	N	331	VAL
3	N	355	VAL
3	N	362	GLU
3	N	372	ASP
3	N	387	LEU

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Mol	Chain	Res	Type
3	N	411	THR
3	N	415	VAL
3	N	421	LEU
3	N	427	VAL
3	N	500	ARG
3	N	548	ILE
3	N	572	ARG
3	N	576	GLU
3	N	586	ARG
3	N	587	ARG
3	N	591	VAL
3	N	618	LEU
3	N	628	ARG
3	N	632	VAL
3	N	646	LYS
3	N	650	LEU
3	N	669	ASN
3	N	675	ARG
3	N	686	GLU
3	N	709	HIS
3	N	754	PHE
3	N	778	LEU
3	N	808	THR
3	N	810	GLU
3	N	817	GLU
3	N	827	ILE
3	N	832	ARG
3	N	864	VAL
3	N	875	THR
3	N	894	LYS
3	N	904	VAL
3	N	907	GLU
3	N	908	LYS
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	1055	VAL
3	N	1062	ARG

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Mol	Chain	Res	Type
3	N	1067	VAL
3	N	1079	LYS
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	1221	VAL
3	N	1277	ILE
3	N	1280	VAL
3	N	1283	ILE
3	N	1313	VAL
3	N	1359	GLN
3	N	1366	LYS
3	N	1382	THR
3	N	1408	ILE
3	N	1444	THR
3	N	1459	LEU
3	N	1468	LEU
3	N	1486	VAL
3	N	1492	LEU
4	O	50	THR
4	O	95	VAL
5	P	78	SER
5	P	88	ILE
5	P	90	GLN
5	P	120	THR
5	P	150	THR
5	P	151	LEU
5	P	156	VAL
5	P	193	ARG
5	P	222	ARG
5	P	277	GLN
5	P	281	GLU
5	P	287	THR
5	P	309	LYS
5	P	310	ILE
5	P	346	THR
5	P	347	GLN
5	P	358	LEU

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Mol	Chain	Res	Type
5	P	360	LYS
5	P	361	LEU
5	P	375	LEU
5	P	376	ILE
5	P	383	LEU
5	P	393	THR
5	P	394	ARG
5	P	400	ILE
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	213	GLN
2	C	117	HIS
2	C	187	ASN
2	C	860	HIS
2	C	991	GLN
3	D	560	GLN
3	D	703	ASN
3	D	994	GLN
3	D	1172	HIS
3	D	1195	GLN
3	D	1359	GLN
3	D	1442	ASN
5	F	175	HIS
5	F	218	GLN
5	F	381	HIS
1	K	213	GLN
2	M	187	ASN

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Mol	Chain	Res	Type
2	M	565	GLN
2	M	860	HIS
2	M	991	GLN
2	M	1047	HIS
3	N	350	HIS
3	N	703	ASN
3	N	994	GLN
3	N	1172	HIS
3	N	1442	ASN
3	N	1445	HIS
5	P	90	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 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, 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	226/315 (71%)	-0.07	2 (0%) 81 75	45, 63, 96, 118	0
1	B	222/315 (70%)	0.21	8 (3%) 46 38	47, 77, 114, 137	0
1	K	226/315 (71%)	-0.04	1 (0%) 88 85	49, 66, 97, 116	0
1	L	225/315 (71%)	0.25	3 (1%) 75 67	51, 81, 118, 139	0
2	C	1111/1119 (99%)	-0.13	6 (0%) 87 83	32, 59, 111, 149	0
2	M	1111/1119 (99%)	0.01	14 (1%) 75 67	34, 65, 129, 152	0
3	D	1486/1524 (97%)	-0.12	11 (0%) 84 79	29, 61, 120, 177	1 (0%)
3	N	1486/1524 (97%)	-0.11	10 (0%) 84 79	32, 64, 118, 178	1 (0%)
4	E	94/99 (94%)	0.10	1 (1%) 78 71	41, 64, 110, 121	0
4	O	94/99 (94%)	-0.10	2 (2%) 63 54	45, 67, 112, 122	0
5	F	346/443 (78%)	-0.08	3 (0%) 81 75	37, 63, 108, 132	0
5	P	347/443 (78%)	0.09	13 (3%) 45 37	42, 72, 139, 172	0
6	G	16/19 (84%)	0.10	1 (6%) 26 20	56, 84, 176, 182	0
6	Q	16/19 (84%)	0.31	2 (12%) 8 7	68, 93, 180, 182	0
7	H	24/27 (88%)	0.25	1 (4%) 40 32	54, 98, 145, 192	0
7	R	24/27 (88%)	0.22	2 (8%) 17 14	55, 112, 147, 199	0
All	All	7054/7722 (91%)	-0.05	80 (1%) 78 71	29, 65, 121, 199	2 (0%)

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	1252	ILE	5.1
3	N	1252	ILE	4.6
2	C	363	SER	4.1
5	P	77	THR	3.6
1	B	190	THR	3.6

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Mol	Chain	Res	Type	RSRZ
4	O	95	VAL	3.4
5	P	139	ALA	3.3
5	P	141	VAL	3.3
5	F	141	VAL	3.1
3	D	595	GLY	3.1
3	D	184	GLU	3.0
5	P	383	LEU	3.0
1	B	7	LYS	2.9
5	P	325	LYS	2.9
1	B	157	GLY	2.8
5	F	139	ALA	2.8
2	M	247	PRO	2.8
1	L	141	GLU	2.8
3	N	184	GLU	2.8
3	D	144	GLY	2.8
3	D	1253	THR	2.8
6	Q	4	DG	2.8
1	L	228	PRO	2.8
2	M	171	TRP	2.8
2	M	311	PHE	2.8
2	M	248	PRO	2.7
6	G	4	DG	2.7
1	B	228	PRO	2.7
2	M	741	GLY	2.7
3	N	1305	LEU	2.7
5	P	392	VAL	2.6
3	N	1280	VAL	2.5
7	H	24	DC	2.5
3	D	175	VAL	2.5
1	B	160	ASP	2.5
5	P	361	LEU	2.5
2	M	152	PRO	2.5
5	F	325	LYS	2.5
1	L	160	ASP	2.4
6	Q	19	DG	2.4
3	N	1270	ALA	2.4
3	N	1253	THR	2.4
3	D	532	GLY	2.4
3	N	1128	VAL	2.4
1	B	186	LEU	2.4
1	B	191	ASP	2.3
2	C	511	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
2	M	245	GLY	2.3
7	R	24	DC	2.3
2	C	764	GLU	2.3
5	P	138	SER	2.3
7	R	12	DC	2.3
1	A	186	LEU	2.3
2	M	102	HIS	2.3
4	E	95	VAL	2.3
3	N	595	GLY	2.3
1	A	188	GLN	2.2
2	M	103	LYS	2.2
1	B	158	ILE	2.2
3	N	486	ARG	2.2
5	P	388	ALA	2.2
3	D	1283	ILE	2.2
2	C	107	LEU	2.2
4	O	51	LEU	2.1
2	M	357	GLU	2.1
5	P	395	GLU	2.1
2	M	1	MET	2.1
3	N	1292	VAL	2.1
5	P	386	VAL	2.1
1	K	187	GLY	2.1
5	P	142	ARG	2.1
2	C	419	THR	2.1
5	P	400	ILE	2.1
2	C	364	GLU	2.1
3	D	1493	LYS	2.0
2	M	44	ILE	2.0
3	D	1277	ILE	2.0
2	M	764	GLU	2.0
2	M	183	SER	2.0
3	D	1502	ALA	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	MG	N	2004	1/1	0.81	0.32	66,66,66,66	0
8	MG	D	2004	1/1	0.83	0.34	66,66,66,66	0
8	MG	P	2001	1/1	0.84	0.18	71,71,71,71	0
8	MG	B	2001	1/1	0.85	0.13	71,71,71,71	0
8	MG	K	1001	1/1	0.85	0.29	67,67,67,67	0
8	MG	N	2005	1/1	0.89	0.11	67,67,67,67	0
8	MG	F	2001	1/1	0.91	0.07	63,63,63,63	0
8	MG	D	2003	1/1	0.93	0.15	32,32,32,32	0
8	MG	N	2003	1/1	0.94	0.15	38,38,38,38	0
8	MG	D	2005	1/1	0.94	0.14	71,71,71,71	0
9	ZN	D	2002	1/1	0.99	0.03	73,73,73,73	0
9	ZN	N	2002	1/1	0.99	0.04	95,95,95,95	0
9	ZN	N	2001	1/1	1.00	0.03	54,54,54,54	0
9	ZN	D	2001	1/1	1.00	0.10	77,77,77,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.