Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2023 – 03:20 AM JST

PDB ID	:	7EH2
Title	:	Thermus thermophilus transcription initiation complex containing a template-strand pyrimidine at position TSS-2 and GpG RNA primer
Authors	:	Li, L.; Zhang, Y.
Deposited on	:	2021-03-27
Resolution	:	3.34 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:

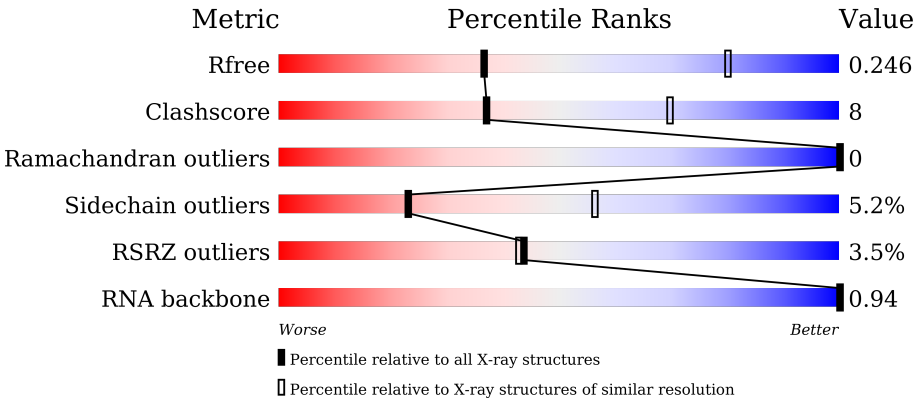
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.34 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}	130704	1060 (3.38-3.30)
Clashscore	141614	1111 (3.38-3.30)
Ramachandran outliers	138981	1090 (3.38-3.30)
Sidechain outliers	138945	1089 (3.38-3.30)
RSRZ outliers	127900	1028 (3.38-3.30)
RNA backbone	3102	1129 (3.78-2.90)

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 <=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	3% 52% 20% • 27%
1	B	315	5% 53% 16% • 30%
1	K	315	6% 54% 16% • 28%
1	L	315	6% 53% 17% • 29%

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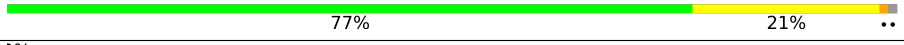
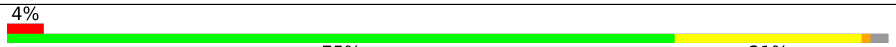
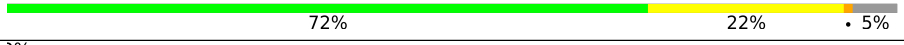
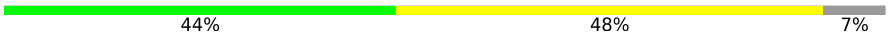
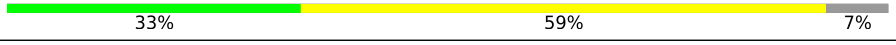
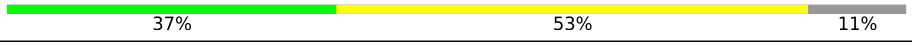
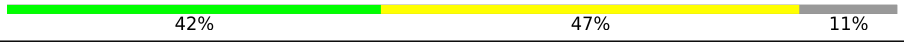
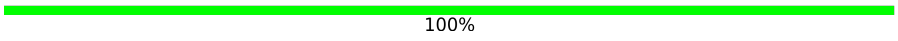
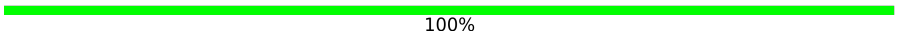
Mol	Chain	Length	Quality of chain
2	C	1119	
2	M	1119	
3	D	1524	
3	N	1524	
4	E	99	
4	O	99	
5	F	443	
5	P	443	
6	G	27	
6	J	27	
7	H	19	
7	Q	19	
8	I	2	
8	R	2	

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 56841 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	229	Total	C	N	O	S	0	0	0
			1777	1136	306	333	2			
1	B	222	Total	C	N	O	S	0	0	0
			1750	1118	304	326	2			
1	K	227	Total	C	N	O	S	0	0	0
			1781	1138	308	333	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
			8742	5534	1552	1632	24			
2	M	1111	Total	C	N	O	S	0	0	0
			8724	5520	1551	1629	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
			11680	7405	2051	2189	35			
3	N	1486	Total	C	N	O	S	0	0	0
			11675	7402	2047	2191	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 SigA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	346	Total	C	N	O	S	0	0	0
			2803	1768	509	522	4			
5	P	347	Total	C	N	O	S	0	0	0
			2757	1738	490	525	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 DNA (27-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	25	Total	C	N	O	P	0	0	0
			516	246	99	147	24			
6	J	25	Total	C	N	O	P	0	0	0
			516	246	99	147	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	17	Total	C	N	O	P	0	0	0
			345	165	63	101	16			
7	Q	17	Total	C	N	O	P	0	0	0
			345	165	63	101	16			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	2	Total	C	N	O	P	0	0	0
			43	20	10	12	1			
8	R	2	Total	C	N	O	P	0	0	0
			43	20	10	12	1			

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

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

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	D	1	Total Mg 1 1	0	0
10	L	1	Total Mg 1 1	0	0
10	N	1	Total Mg 1 1	0	0

- Molecule 11 is water.

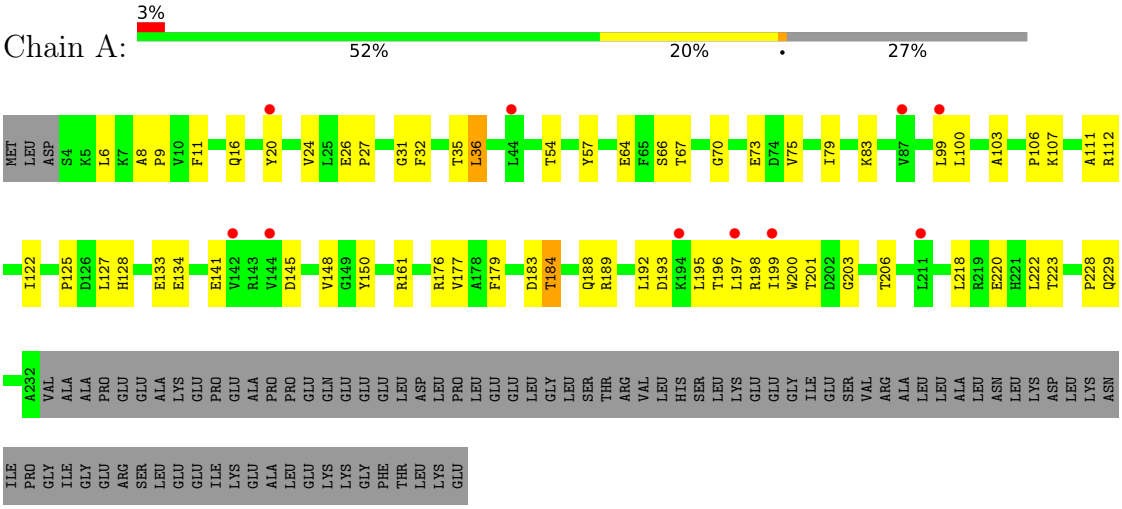
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	4	Total O 4 4	0	0
11	B	4	Total O 4 4	0	0
11	C	5	Total O 5 5	0	0
11	D	10	Total O 10 10	0	0
11	E	2	Total O 2 2	0	0
11	F	1	Total O 1 1	0	0
11	K	2	Total O 2 2	0	0
11	L	1	Total O 1 1	0	0
11	M	1	Total O 1 1	0	0
11	N	9	Total O 9 9	0	0
11	O	2	Total O 2 2	0	0
11	G	1	Total O 1 1	0	0

3 Residue-property plots (i)

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.

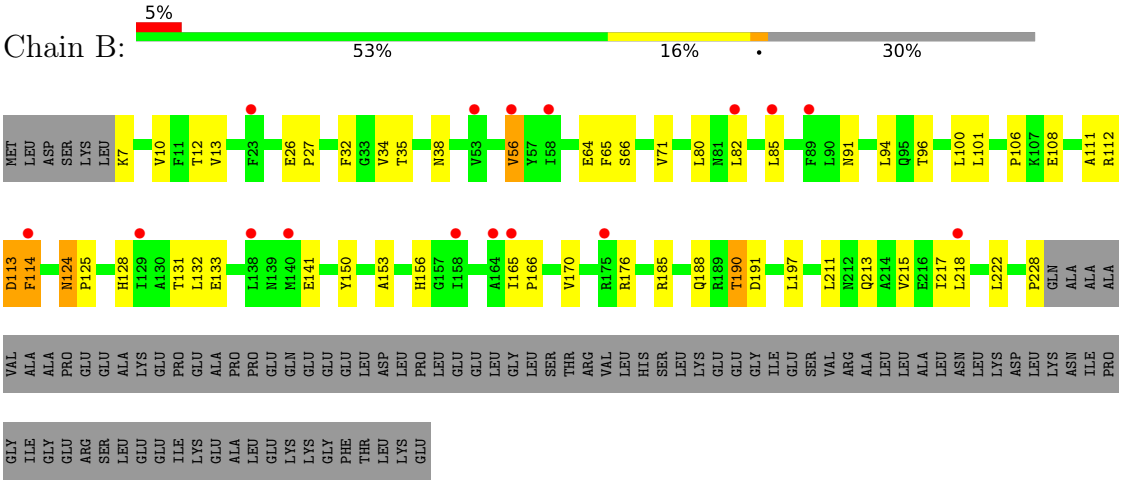
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:



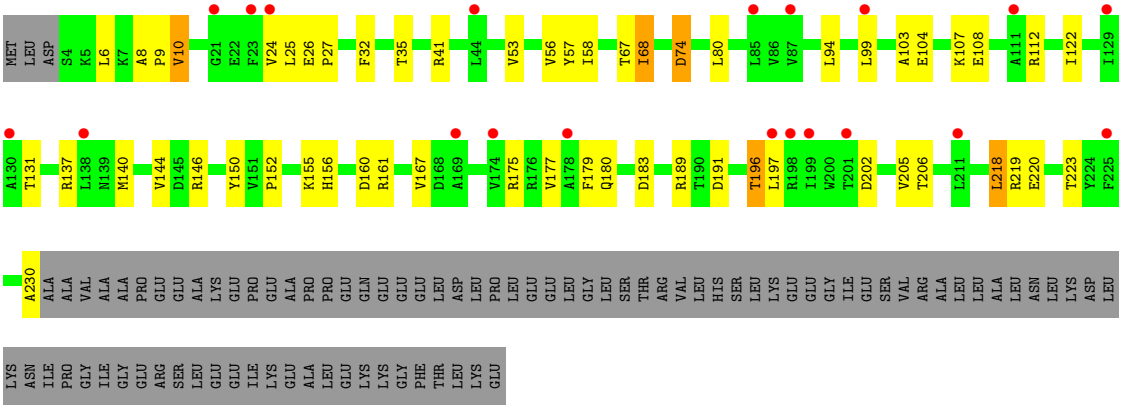
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain B:



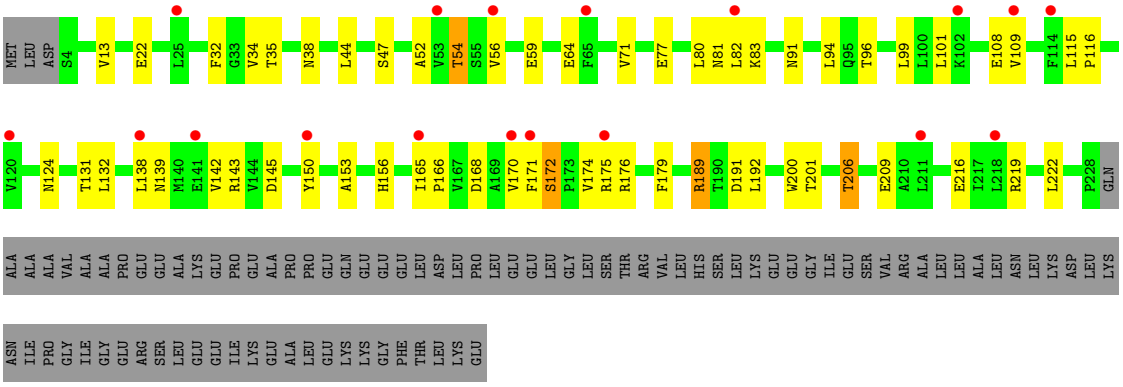
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain K:



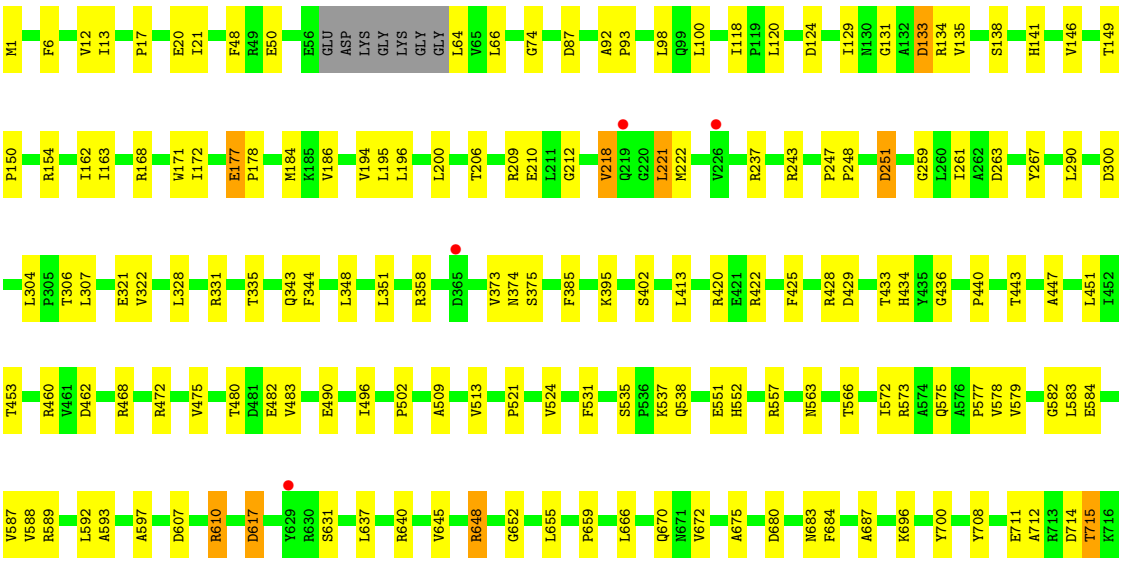
• Molecule 1: DNA-directed RNA polymerase subunit alpha

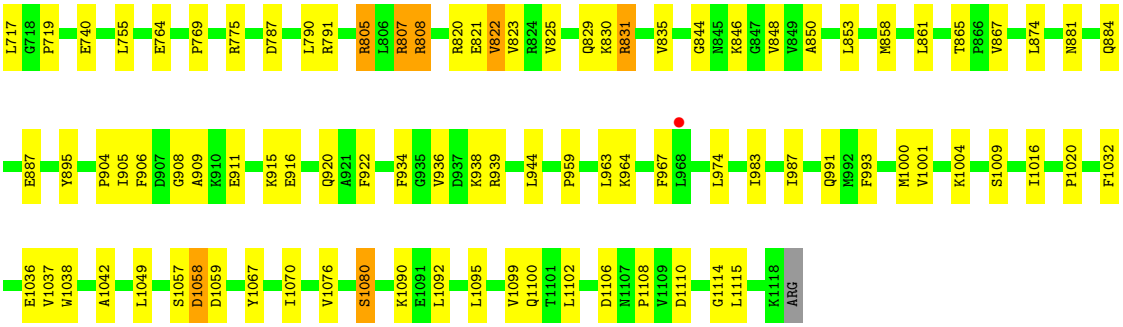
Chain L:



• Molecule 2: DNA-directed RNA polymerase subunit beta

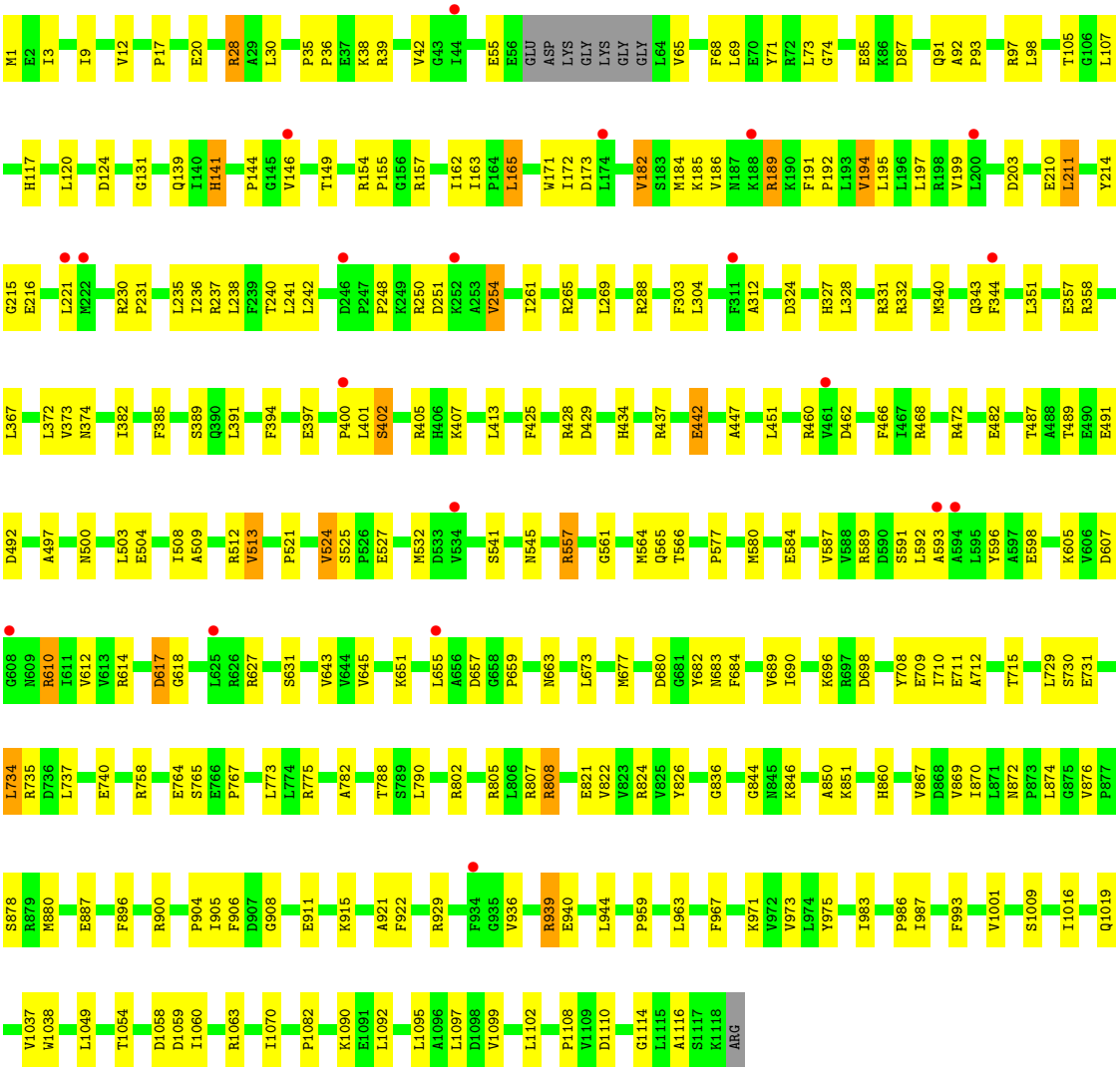
Chain C:





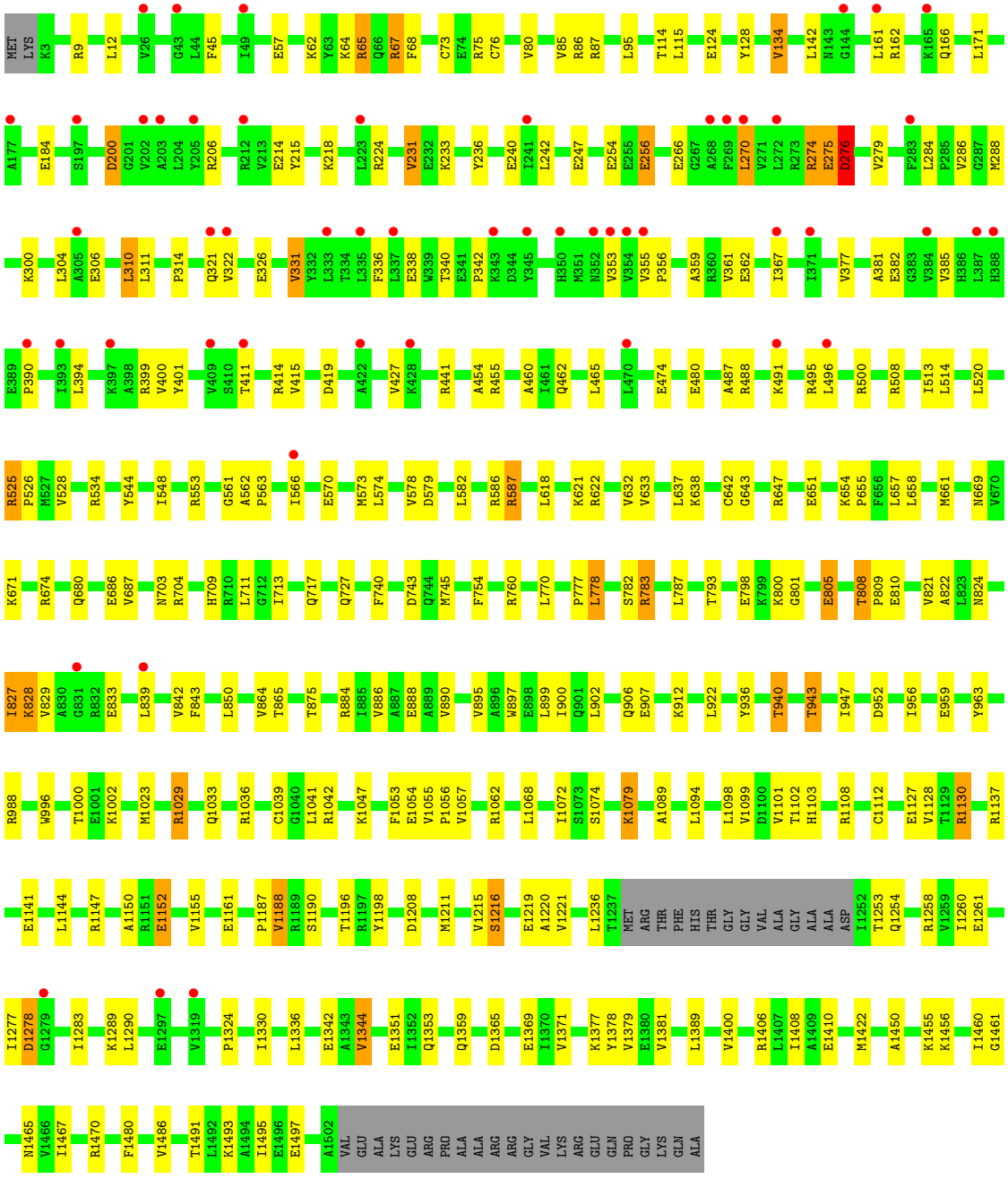
• Molecule 2: DNA-directed RNA polymerase subunit beta

Chain M:

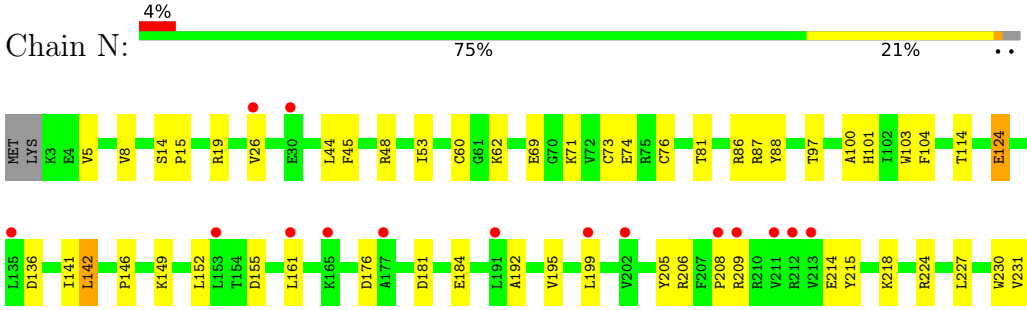


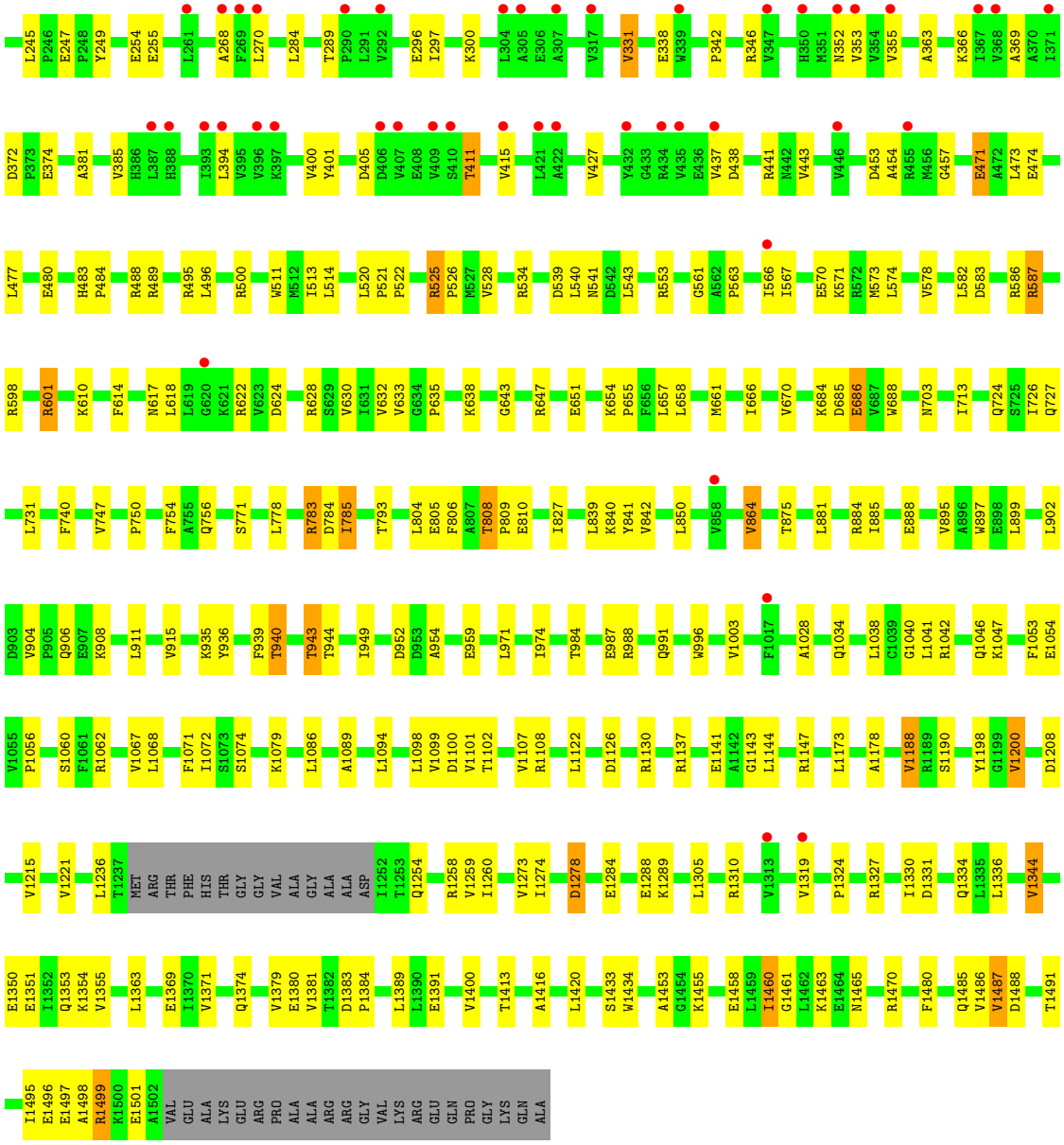
• Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain D:



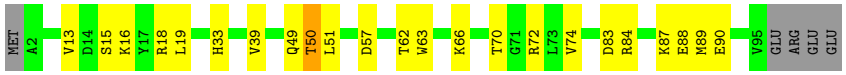
• Molecule 3: DNA-directed RNA polymerase subunit beta'





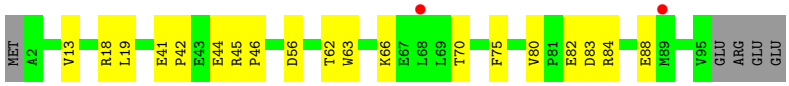
• Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E:



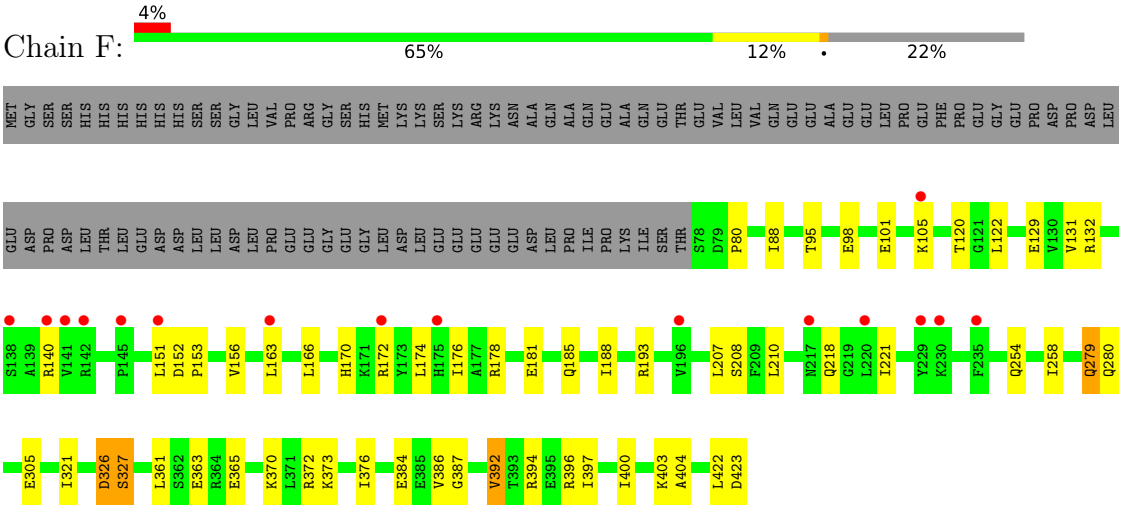
• Molecule 4: DNA-directed RNA polymerase subunit omega

Chain O:



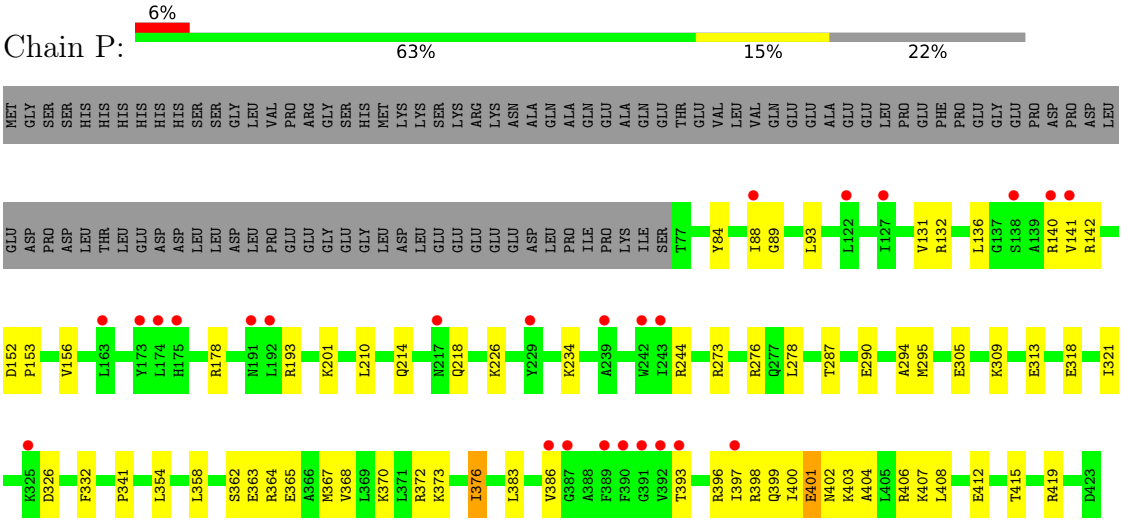
• Molecule 5: RNA polymerase sigma factor SigA

Chain F:



• Molecule 5: RNA polymerase sigma factor SigA

Chain P:

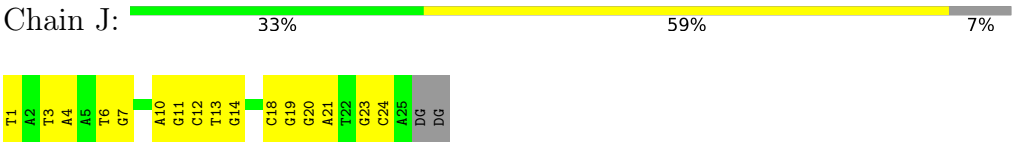


• Molecule 6: DNA (27-MER)

Chain G:

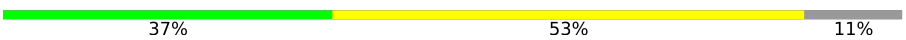
• Molecule 6: DNA (27-MER)

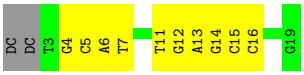
Chain J:



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

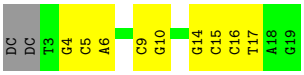
Chain H:





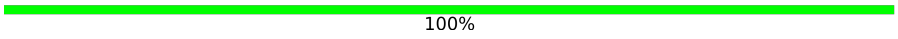
• Molecule 7: DNA (5'-D(*CP*C*TP*GP*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*CP*CP*TP*AP*G)-3')

Chain Q:



• Molecule 8: RNA (5'-R(*GP*G)-3')

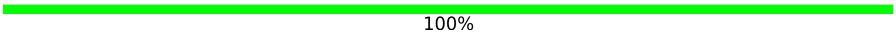
Chain I:



There are no outlier residues recorded for this chain.

• Molecule 8: RNA (5'-R(*GP*G)-3')

Chain R:



There are no outlier residues recorded for this chain.

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	184.85Å 104.20Å 296.65Å 90.00° 98.42° 90.00°	Depositor
Resolution (Å)	97.82 – 3.34 123.62 – 3.34	Depositor EDS
% Data completeness (in resolution range)	99.3 (97.82-3.34) 99.6 (123.62-3.34)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.35 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.201 , 0.247 0.201 , 0.246	Depositor DCC
R_{free} test set	8256 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	88.8	Xtriage
Anisotropy	0.666	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 59.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	56841	wwPDB-VP
Average B, all atoms (Å^2)	96.0	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 38.14 % 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 3.8581e-04. 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.25	0/1809	0.46	0/2464
1	B	0.25	0/1782	0.45	0/2424
1	K	0.26	0/1813	0.47	0/2466
1	L	0.26	0/1805	0.47	0/2454
2	C	0.26	0/8909	0.44	0/12054
2	M	0.26	0/8890	0.45	1/12030 (0.0%)
3	D	0.25	0/11885	0.44	0/16081
3	N	0.25	0/11880	0.44	0/16074
4	E	0.24	0/775	0.41	0/1045
4	O	0.25	0/775	0.40	0/1045
5	F	0.25	0/2848	0.41	0/3832
5	P	0.25	0/2800	0.41	0/3777
6	G	0.54	0/580	0.93	0/895
6	J	0.55	0/580	0.95	0/895
7	H	0.56	0/386	0.92	0/594
7	Q	0.54	0/386	0.90	0/594
8	I	0.30	0/48	0.92	0/74
8	R	0.35	0/48	1.06	0/74
All	All	0.27	0/57999	0.47	1/78872 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	D	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	211	LEU	CA-CB-CG	5.03	126.88	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	274	ARG	Peptide
3	D	276	ASP	Peptide

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	1777	0	1812	42	0
1	B	1750	0	1797	31	0
1	K	1781	0	1828	32	0
1	L	1773	0	1826	35	0
2	C	8742	0	8826	138	0
2	M	8724	0	8795	165	0
3	D	11680	0	11864	187	0
3	N	11675	0	11851	203	0
4	E	761	0	778	14	0
4	O	761	0	778	12	0
5	F	2803	0	2878	39	0
5	P	2757	0	2780	47	0
6	G	516	0	283	10	0
6	J	516	0	283	15	0
7	H	345	0	193	9	0
7	Q	345	0	193	10	0
8	I	43	0	23	0	0
8	R	43	0	23	0	0
9	D	2	0	0	0	0
9	N	2	0	0	0	0
10	D	1	0	0	0	0
10	L	1	0	0	0	0
10	N	1	0	0	0	0
11	A	4	0	0	0	0
11	B	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	C	5	0	0	0	0
11	D	10	0	0	0	0
11	E	2	0	0	0	0
11	F	1	0	0	0	0
11	G	1	0	0	0	0
11	K	2	0	0	0	0
11	L	1	0	0	0	0
11	M	1	0	0	0	0
11	N	9	0	0	3	0
11	O	2	0	0	0	0
All	All	56841	0	56811	882	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 (882) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:462:ASP:HB3	2:M:468:ARG:HD2	1.58	0.84
3:N:1495:ILE:HD13	4:O:80:VAL:HG21	1.62	0.81
2:M:683:ASN:HB3	2:M:872:ASN:HB2	1.61	0.81
5:P:408:LEU:O	5:P:412:GLU:HB2	1.83	0.77
3:N:60:CYS:SG	11:N:1702:HOH:O	2.43	0.76
3:D:1112:CYS:HB3	3:D:1196:THR:HG23	1.67	0.75
3:N:142:LEU:HB2	3:N:161:LEU:HD21	1.68	0.74
2:M:154:ARG:HE	2:M:157:ARG:HG3	1.50	0.74
1:B:108:GLU:HG2	1:B:131:THR:HG22	1.71	0.72
3:N:73:CYS:SG	11:N:1702:HOH:O	2.47	0.72
3:D:124:GLU:OE2	3:D:587:ARG:NH2	2.23	0.71
2:M:689:VAL:HG13	2:M:851:LYS:HB3	1.72	0.71
1:A:24:VAL:HG22	1:A:196:THR:HG23	1.72	0.71
1:L:56:VAL:HG21	1:L:82:LEU:HD13	1.73	0.71
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.73	0.71
1:B:32:PHE:HA	1:B:35:THR:HB	1.72	0.70
3:N:1324:PRO:HG3	3:N:1330:ILE:HD11	1.72	0.70
2:M:557:ARG:HG3	2:M:844:GLY:HA3	1.74	0.70
3:N:520:LEU:HD23	3:N:525:ARG:HG2	1.74	0.69
2:M:428:ARG:NH2	2:M:447:ALA:O	2.24	0.69
3:D:162:ARG:O	3:D:414:ARG:NH1	2.26	0.69
3:D:270:LEU:HD12	3:D:284:LEU:HD11	1.75	0.69
1:B:71:VAL:HG22	1:B:132:LEU:HG	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:802:ARG:HB2	2:M:826:TYR:HB2	1.73	0.68
3:D:256:GLU:O	3:D:274:ARG:NH2	2.25	0.68
2:C:428:ARG:NH2	2:C:447:ALA:O	2.27	0.68
2:C:1115:LEU:HB3	3:D:85:VAL:HG12	1.76	0.68
5:P:136:LEU:HD13	5:P:140:ARG:HG2	1.76	0.68
2:C:462:ASP:HB3	2:C:468:ARG:HD2	1.76	0.68
3:N:1498:ALA:HB1	4:O:84:ARG:HH21	1.58	0.68
2:C:829:GLN:OE1	2:C:831:ARG:NH2	2.26	0.68
2:M:172:ILE:HG13	2:M:186:VAL:HG22	1.76	0.67
2:M:577:PRO:HG2	2:M:580:MET:HG2	1.77	0.67
3:D:1254:GLN:HB3	3:D:1258:ARG:HB2	1.76	0.67
2:M:773:LEU:HD23	5:P:354:LEU:HD13	1.77	0.67
5:P:354:LEU:O	5:P:358:LEU:HB2	1.94	0.67
2:M:905:ILE:HG23	2:M:906:PHE:HD1	1.60	0.67
2:C:343:GLN:HG3	2:C:385:PHE:HB2	1.76	0.66
3:D:809:PRO:HB3	3:D:839:LEU:HD13	1.76	0.66
2:M:189:ARG:HH12	2:M:242:LEU:HA	1.58	0.66
2:M:874:LEU:HD13	3:N:783:ARG:HB2	1.78	0.66
6:J:3:DT:H2'	6:J:4:DA:C8	2.30	0.66
1:B:111:ALA:HB3	1:B:125:PRO:HA	1.76	0.66
1:L:32:PHE:HA	1:L:35:THR:HB	1.76	0.66
3:N:1480:PHE:O	4:O:18:ARG:NH2	2.29	0.66
3:D:1033:GLN:OE1	3:D:1036:ARG:NH1	2.29	0.66
3:N:750:PRO:O	3:N:756:GLN:NE2	2.30	0.65
2:M:680:ASP:H	3:N:943:THR:CG2	2.08	0.65
2:C:787:ASP:OD2	2:C:791:ARG:NH2	2.30	0.65
3:D:798:GLU:HG3	3:D:824:ASN:HB2	1.78	0.65
3:N:984:THR:HG22	3:N:987:GLU:HG3	1.77	0.65
5:F:153:PRO:HA	5:F:156:VAL:HG22	1.78	0.65
2:C:915:LYS:NZ	3:D:952:ASP:OD2	2.28	0.65
2:M:144:PRO:HG2	2:M:165:LEU:HD23	1.78	0.64
3:D:142:LEU:HB2	3:D:161:LEU:HD21	1.80	0.64
3:N:218:LYS:HG2	3:N:338:GLU:HG2	1.79	0.64
1:B:112:ARG:HG3	1:B:125:PRO:HB2	1.79	0.64
5:F:400:ILE:HA	5:F:403:LYS:HG2	1.79	0.64
2:M:876:VAL:HB	3:N:949:ILE:HD12	1.80	0.64
3:D:326:GLU:HG2	3:D:331:VAL:HG13	1.80	0.63
5:P:273:ARG:HG2	5:P:276:ARG:HH12	1.64	0.63
2:C:200:LEU:HD13	2:C:300:ASP:HB2	1.81	0.63
3:N:224:ARG:NE	3:N:254:GLU:OE2	2.31	0.62
2:C:905:ILE:HG23	2:C:906:PHE:HD2	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:988:ARG:NH2	3:D:1054:GLU:OE2	2.31	0.62
1:K:9:PRO:HB3	1:K:27:PRO:HD2	1.82	0.62
1:K:104:GLU:OE2	1:K:137:ARG:NH1	2.33	0.62
2:M:983:ILE:HG21	2:M:987:ILE:HD11	1.79	0.62
2:C:617:ASP:OD1	2:C:617:ASP:N	2.32	0.62
3:N:1108:ARG:NH2	3:N:1198:TYR:O	2.33	0.62
2:C:911:GLU:O	2:C:915:LYS:HG2	2.00	0.62
5:P:370:LYS:HB3	5:P:376:ILE:HD13	1.81	0.62
3:D:455:ARG:HB2	3:D:460:ALA:HB2	1.82	0.62
5:F:397:ILE:HD13	5:F:400:ILE:HD11	1.82	0.62
1:L:206:THR:HG22	1:L:209:GLU:H	1.63	0.62
3:N:685:ASP:HA	3:N:688:TRP:HD1	1.64	0.62
2:M:684:PHE:HB3	3:N:633:VAL:HG21	1.81	0.61
2:M:397:GLU:HG3	2:M:631:SER:HB2	1.82	0.61
3:D:520:LEU:O	3:D:525:ARG:NH1	2.32	0.61
1:K:24:VAL:HG22	1:K:196:THR:HG23	1.83	0.61
1:K:32:PHE:HA	1:K:35:THR:HB	1.82	0.61
2:M:521:PRO:HB3	3:N:1068:LEU:HD21	1.83	0.61
3:N:270:LEU:HG	3:N:284:LEU:HD11	1.81	0.61
1:A:99:LEU:HD21	1:A:122:ILE:HD11	1.83	0.61
7:H:15:DC:H2'	7:H:16:DC:C6	2.36	0.61
6:J:23:DG:H2"	6:J:24:DC:H5"	1.83	0.61
3:N:1101:VAL:HG13	3:N:1102:THR:HG23	1.83	0.61
1:B:153:ALA:HA	1:B:156:HIS:CD2	2.36	0.61
3:N:771:SER:HB2	3:N:778:LEU:HG	1.82	0.60
2:C:684:PHE:HB3	3:D:633:VAL:HG21	1.82	0.60
2:C:805:ARG:HG3	2:C:823:VAL:HG22	1.84	0.60
2:C:874:LEU:HD13	3:D:783:ARG:HB2	1.82	0.60
2:M:92:ALA:HB2	2:M:120:LEU:HD11	1.84	0.60
1:A:32:PHE:HA	1:A:35:THR:HB	1.84	0.60
2:M:758:ARG:HH21	2:M:788:THR:HB	1.66	0.60
3:N:534:ARG:NH2	5:P:313:GLU:O	2.35	0.60
3:D:256:GLU:HG3	3:D:300:LYS:HG3	1.84	0.60
3:N:1254:GLN:HB3	3:N:1258:ARG:HB2	1.84	0.59
7:H:15:DC:H2'	7:H:16:DC:H6	1.67	0.59
1:A:9:PRO:HB3	1:A:27:PRO:HD2	1.85	0.59
4:E:39:VAL:O	4:E:72:ARG:NH1	2.31	0.59
2:C:50:GLU:OE2	2:C:168:ARG:NH1	2.35	0.59
3:N:366:LYS:HD3	3:N:369:ALA:HB2	1.84	0.59
3:D:288:MET:HA	3:D:306:GLU:O	2.02	0.59
2:M:182:VAL:HG13	2:M:221:LEU:HD13	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:403:LYS:HA	5:P:406:ARG:HG2	1.84	0.59
3:D:1152:GLU:HG2	3:D:1161:GLU:HA	1.84	0.59
6:J:12:DC:H4'	6:J:13:DT:H5'	1.84	0.59
1:A:179:PHE:HB3	1:A:197:LEU:HD23	1.85	0.59
2:M:915:LYS:NZ	3:N:952:ASP:OD2	2.34	0.59
5:F:163:LEU:HD13	5:F:174:LEU:HD13	1.84	0.59
1:K:179:PHE:HB3	1:K:197:LEU:HD23	1.83	0.59
3:N:480:GLU:OE2	3:N:488:ARG:NH2	2.35	0.59
3:N:793:THR:HG21	3:N:906:GLN:HG2	1.85	0.59
5:P:131:VAL:HG13	5:P:178:ARG:HD3	1.83	0.59
3:N:785:ILE:HD12	3:N:935:LYS:HA	1.85	0.59
3:D:171:LEU:HD22	3:D:390:PRO:HG2	1.85	0.59
5:F:188:ILE:HD13	5:F:221:ILE:HG12	1.85	0.59
2:C:916:GLU:OE1	2:C:920:GLN:NE2	2.32	0.59
3:N:1003:VAL:HG21	3:N:1041:LEU:HG	1.85	0.59
1:A:26:GLU:HB3	1:A:27:PRO:HD3	1.85	0.58
5:P:226:LYS:HD3	6:J:1:DT:H73	1.85	0.58
5:P:362:SER:HB3	5:P:365:GLU:HG3	1.85	0.58
7:Q:14:DG:H2'	7:Q:15:DC:H6	1.67	0.58
2:M:87:ASP:HA	2:M:131:GLY:HA3	1.84	0.58
2:C:808:ARG:NH2	5:F:305:GLU:OE2	2.35	0.58
2:C:64:LEU:HD22	2:C:100:LEU:HD11	1.85	0.58
3:N:400:VAL:HG13	3:N:443:VAL:HG21	1.84	0.58
2:C:769:PRO:HG3	3:D:65:ARG:HH11	1.67	0.58
2:C:1067:TYR:OH	3:D:674:ARG:NH1	2.37	0.58
2:M:55:GLU:HA	2:M:65:VAL:HG22	1.86	0.58
2:M:711:GLU:HG2	2:M:822:VAL:HG22	1.86	0.58
2:M:1054:THR:HG22	2:M:1082:PRO:HG3	1.85	0.58
5:F:386:VAL:HB	5:F:397:ILE:HG21	1.85	0.58
2:M:971:LYS:HB3	2:M:986:PRO:HB2	1.86	0.58
3:D:1258:ARG:HH21	3:D:1351:GLU:HG2	1.68	0.57
2:M:936:VAL:HG11	2:M:959:PRO:HB2	1.86	0.57
2:M:614:ARG:NH2	2:M:618:GLY:O	2.37	0.57
3:D:480:GLU:OE2	3:D:488:ARG:NH2	2.37	0.57
3:N:601:ARG:HD3	5:P:318:GLU:HG2	1.86	0.57
3:D:57:GLU:HG3	3:D:64:LYS:HG2	1.86	0.57
4:E:50:THR:OG1	4:E:51:LEU:N	2.37	0.57
3:D:1102:THR:HG21	3:D:1371:VAL:HG22	1.86	0.57
3:D:1236:LEU:HA	3:D:1359:GLN:HG3	1.87	0.57
2:C:420:ARG:HD3	2:C:447:ALA:HB1	1.87	0.56
3:D:1208:ASP:HB2	3:D:1215:VAL:HA	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:513:VAL:HG22	2:M:524:VAL:HG12	1.86	0.56
4:E:57:ASP:O	4:E:63:TRP:NE1	2.35	0.56
3:D:1101:VAL:HG13	3:D:1102:THR:HG23	1.88	0.56
3:D:1324:PRO:HG3	3:D:1330:ILE:HD11	1.87	0.56
5:F:326:ASP:OD1	5:F:326:ASP:N	2.34	0.56
1:K:94:LEU:O	1:K:146:ARG:NH1	2.36	0.56
2:M:593:ALA:HB1	2:M:659:PRO:HD2	1.87	0.56
5:F:166:LEU:HD13	5:F:170:HIS:HB3	1.88	0.56
1:L:175:ARG:N	1:L:200:TRP:O	2.32	0.56
5:P:140:ARG:HG3	5:P:142:ARG:HH22	1.71	0.56
6:G:12:DC:H4'	6:G:13:DT:H5'	1.88	0.56
1:B:113:ASP:OD1	1:B:113:ASP:N	2.39	0.56
1:L:101:LEU:HD21	1:L:109:VAL:HG11	1.88	0.55
1:L:153:ALA:HB1	1:L:166:PRO:HB2	1.88	0.55
2:M:195:LEU:HD23	2:M:238:LEU:HD13	1.86	0.55
2:C:904:PRO:HD2	2:C:908:GLY:HA2	1.87	0.55
1:L:153:ALA:HA	1:L:156:HIS:CD2	2.42	0.55
5:P:396:ARG:HH21	5:P:400:ILE:HD12	1.69	0.55
3:D:805:GLU:OE2	3:D:828:LYS:NZ	2.31	0.55
1:L:91:ASN:HB3	1:L:94:LEU:HB2	1.87	0.55
3:N:1102:THR:HG21	3:N:1371:VAL:HG22	1.89	0.55
3:N:1137:ARG:O	3:N:1141:GLU:HG3	2.07	0.55
6:J:10:DA:H2"	6:J:11:DG:C8	2.42	0.55
2:C:1092:LEU:HD13	2:C:1099:VAL:HG21	1.89	0.55
3:N:124:GLU:OE2	3:N:587:ARG:NH2	2.39	0.55
1:K:74:ASP:HB3	2:M:627:ARG:HH12	1.72	0.55
2:M:12:VAL:HG21	2:M:472:ARG:HD3	1.89	0.55
3:N:574:LEU:O	3:N:578:VAL:HG23	2.06	0.55
6:G:23:DG:H2"	6:G:24:DC:H5"	1.88	0.55
3:N:1274:ILE:HG22	3:N:1324:PRO:HA	1.88	0.55
3:D:520:LEU:HD23	3:D:525:ARG:HG2	1.89	0.54
1:K:74:ASP:OD1	1:K:74:ASP:N	2.37	0.54
3:N:231:VAL:O	3:N:236:TYR:OH	2.20	0.54
2:M:617:ASP:OD1	2:M:617:ASP:N	2.40	0.54
2:M:680:ASP:H	3:N:943:THR:HG21	1.72	0.54
1:B:100:LEU:HG	1:B:141:GLU:HG2	1.90	0.54
2:C:92:ALA:HB2	2:C:120:LEU:HD11	1.89	0.54
3:D:553:ARG:HD2	3:D:570:GLU:OE2	2.08	0.54
2:M:680:ASP:H	3:N:943:THR:HG22	1.71	0.54
7:Q:14:DG:H2'	7:Q:15:DC:C6	2.41	0.54
2:C:129:ILE:HB	2:C:134:ARG:HD2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:988:ARG:NH2	3:N:1054:GLU:OE2	2.38	0.54
2:C:1059:ASP:OD2	2:C:1080:SER:N	2.39	0.54
3:D:1108:ARG:NH2	3:D:1198:TYR:O	2.40	0.54
1:B:128:HIS:CE1	1:B:131:THR:HG23	2.43	0.54
1:L:176:ARG:NH2	3:N:888:GLU:OE1	2.40	0.54
2:M:904:PRO:HD2	2:M:908:GLY:HA2	1.88	0.54
1:B:56:VAL:HG21	1:B:82:LEU:HD13	1.89	0.54
3:D:356:PRO:HG2	3:D:359:ALA:HB2	1.90	0.54
3:D:1336:LEU:HB2	3:D:1344:VAL:HG21	1.89	0.54
3:N:1208:ASP:HB2	3:N:1215:VAL:HA	1.90	0.54
2:C:12:VAL:HG11	2:C:472:ARG:HD3	1.90	0.54
3:N:632:VAL:N	3:N:726:ILE:O	2.40	0.54
6:J:18:DC:H2"	6:J:19:DG:C8	2.43	0.54
2:C:17:PRO:HB2	2:C:20:GLU:HB3	1.88	0.54
2:C:1038:TRP:CE2	3:D:1099:VAL:HG11	2.42	0.54
3:N:633:VAL:HG13	3:N:635:PRO:HD3	1.88	0.54
3:D:275:GLU:HG2	3:D:276:ASP:N	2.23	0.54
3:D:355:VAL:HG11	3:D:385:VAL:HG21	1.90	0.54
3:D:782:SER:OG	3:D:783:ARG:N	2.41	0.54
2:M:911:GLU:O	2:M:915:LYS:HG2	2.08	0.54
7:Q:15:DC:H2'	7:Q:16:DC:H6	1.73	0.53
1:L:71:VAL:HG22	1:L:132:LEU:HG	1.90	0.53
5:F:131:VAL:HG13	5:F:178:ARG:HD3	1.90	0.53
1:L:52:ALA:HB2	1:L:171:PHE:HA	1.89	0.53
1:L:99:LEU:HB2	1:L:142:VAL:HG22	1.90	0.53
3:D:657:LEU:HG	3:D:661:MET:HE2	1.89	0.53
3:N:1100:ASP:OD2	3:N:1463:LYS:NZ	2.34	0.53
3:D:1450:ALA:HA	3:D:1455:LYS:HD2	1.91	0.53
1:A:70:GLY:N	2:C:607:ASP:OD1	2.42	0.53
2:C:850:ALA:HB1	3:D:633:VAL:HG12	1.90	0.53
2:C:1095:LEU:HD23	3:D:582:LEU:HD22	1.90	0.53
3:D:233:LYS:NZ	3:D:240:GLU:OE2	2.28	0.53
3:N:809:PRO:HB3	3:N:839:LEU:HD13	1.91	0.53
5:P:193:ARG:HB2	6:J:6:DT:H1'	1.89	0.53
5:F:365:GLU:HB2	5:F:404:ALA:HB2	1.91	0.53
2:C:133:ASP:HB3	2:C:395:LYS:HE3	1.90	0.53
2:C:146:VAL:HG22	2:C:162:ILE:HG12	1.91	0.53
2:C:331:ARG:NH2	6:G:14:DG:O6	2.42	0.53
3:D:562:ALA:O	5:F:140:ARG:NH1	2.28	0.53
3:D:1480:PHE:O	4:E:18:ARG:NH2	2.42	0.53
2:C:572:ILE:HG13	2:C:573:ARG:HG3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:587:VAL:HG11	2:C:666:LEU:HD22	1.91	0.53
2:M:331:ARG:NH2	6:J:14:DG:O6	2.41	0.53
3:N:808:THR:HB	3:N:810:GLU:HG2	1.91	0.53
3:N:850:LEU:HD12	3:N:884:ARG:NH2	2.24	0.53
5:P:365:GLU:HA	5:P:368:VAL:HG22	1.91	0.53
3:D:671:LYS:NZ	5:F:423:ASP:OD1	2.40	0.52
2:M:69:LEU:HD12	2:M:97:ARG:HG2	1.91	0.52
3:N:134:VAL:HG12	3:N:454:ALA:HB2	1.91	0.52
3:N:1495:ILE:HG12	4:O:88:GLU:HG3	1.91	0.52
2:C:578:VAL:HG23	2:C:579:VAL:HG23	1.91	0.52
2:M:413:LEU:HD21	2:M:451:LEU:HD13	1.92	0.52
1:B:124:ASN:OD1	1:B:124:ASN:N	2.41	0.52
3:D:704:ARG:HB2	3:D:745:MET:HG2	1.90	0.52
3:N:1258:ARG:HH21	3:N:1351:GLU:HG2	1.72	0.52
2:C:135:VAL:HG23	2:C:395:LYS:HG3	1.91	0.52
2:C:1009:SER:HB3	3:D:651:GLU:O	2.08	0.52
3:D:890:VAL:HB	3:D:922:LEU:HD22	1.92	0.52
3:D:1353:GLN:NE2	3:D:1365:ASP:OD1	2.42	0.52
2:M:171:TRP:CH2	6:J:14:DG:H5'	2.45	0.52
3:D:633:VAL:HA	3:D:740:PHE:CZ	2.45	0.52
2:M:607:ASP:HB2	2:M:610:ARG:NH1	2.25	0.52
3:N:1353:GLN:NE2	3:N:1363:LEU:O	2.38	0.52
5:P:326:ASP:OD1	5:P:326:ASP:N	2.39	0.52
2:M:351:LEU:HD21	2:M:373:VAL:HG13	1.92	0.52
2:M:710:ILE:HD12	2:M:790:LEU:HB2	1.91	0.52
2:M:1038:TRP:CE2	3:N:1099:VAL:HG11	2.45	0.52
2:M:1095:LEU:HD23	3:N:582:LEU:HD22	1.91	0.52
3:N:45:PHE:O	3:N:86:ARG:NH2	2.42	0.52
3:D:1495:ILE:HG12	4:E:88:GLU:HG3	1.92	0.52
2:M:836:GLY:HA3	2:M:1001:VAL:HG21	1.90	0.52
6:G:3:DT:H2"	6:G:4:DA:C8	2.45	0.52
6:J:20:DG:H2"	6:J:21:DA:C8	2.45	0.52
1:B:64:GLU:HA	1:B:165:ILE:HD13	1.90	0.51
1:K:26:GLU:HB3	1:K:27:PRO:HD3	1.91	0.51
7:H:5:DC:H2'	7:H:6:DA:C8	2.45	0.51
3:N:401:TYR:HB3	3:N:427:VAL:HG21	1.93	0.51
3:N:1485:GLN:O	4:O:75:PHE:HA	2.11	0.51
1:K:10:VAL:HG22	1:K:26:GLU:HB3	1.92	0.51
2:M:269:LEU:O	2:M:288:ARG:HD2	2.10	0.51
3:N:1107:VAL:HA	3:N:1200:VAL:O	2.10	0.51
3:D:242:LEU:HB3	3:D:311:LEU:HD12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:526:PRO:HB2	3:D:528:VAL:HG13	1.91	0.51
3:N:996:TRP:CD2	3:N:1056:PRO:HG3	2.45	0.51
6:G:24:DC:H2'	6:G:25:DA:C8	2.45	0.51
1:L:143:ARG:NE	1:L:145:ASP:OD1	2.44	0.51
3:N:657:LEU:HG	3:N:661:MET:HE2	1.93	0.51
4:O:66:LYS:O	4:O:70:THR:HG23	2.10	0.51
2:C:936:VAL:HG11	2:C:959:PRO:HB2	1.93	0.51
5:P:278:LEU:HD11	5:P:294:ALA:HB3	1.92	0.51
2:M:327:HIS:NE2	2:M:492:ASP:OD2	2.36	0.51
5:P:152:ASP:OD1	5:P:152:ASP:N	2.42	0.51
2:C:172:ILE:HG12	2:C:186:VAL:HG22	1.93	0.51
2:C:413:LEU:HD21	2:C:451:LEU:HD13	1.92	0.51
2:C:521:PRO:HB3	3:D:1068:LEU:HD21	1.93	0.51
3:N:806:PHE:CD1	3:N:827:ILE:HD11	2.46	0.51
3:N:911:LEU:O	3:N:915:VAL:HG23	2.11	0.51
2:M:504:GLU:HG2	2:M:509:ALA:HB2	1.92	0.51
3:N:897:TRP:CH2	3:N:902:LEU:HD22	2.46	0.51
7:Q:15:DC:H2'	7:Q:16:DC:C6	2.46	0.51
2:M:324:ASP:HB3	2:M:327:HIS:HB2	1.91	0.50
2:M:673:LEU:HD23	2:M:867:VAL:HA	1.93	0.50
6:J:18:DC:H2"	6:J:19:DG:H8	1.75	0.50
1:B:176:ARG:NH2	3:D:888:GLU:OE1	2.44	0.50
2:C:551:GLU:HG2	2:C:552:HIS:CD2	2.47	0.50
3:D:321:GLN:HB2	3:D:336:PHE:HD2	1.77	0.50
1:K:99:LEU:HD21	1:K:122:ILE:HD11	1.93	0.50
3:N:489:ARG:NH1	3:N:1391:GLU:OE2	2.44	0.50
6:J:11:DG:H2'	6:J:12:DC:C4	2.45	0.50
3:D:793:THR:HG21	3:D:906:GLN:HG2	1.94	0.50
1:A:177:VAL:HG22	1:A:199:ILE:HG12	1.93	0.50
3:D:637:LEU:HD13	3:D:642:CYS:HA	1.92	0.50
2:M:184:MET:HG2	2:M:186:VAL:HG23	1.92	0.50
3:N:45:PHE:CD2	3:N:522:PRO:HB3	2.47	0.50
3:N:1381:VAL:HG21	3:N:1389:LEU:HD23	1.94	0.50
3:D:821:VAL:HG11	3:D:827:ILE:HD11	1.94	0.50
2:M:194:VAL:HA	2:M:197:LEU:HD12	1.93	0.50
3:D:1144:LEU:O	3:D:1147:ARG:HG3	2.11	0.50
2:M:343:GLN:HG3	2:M:385:PHE:HB2	1.93	0.50
2:M:405:ARG:HD2	2:M:442:GLU:OE2	2.12	0.50
3:N:411:THR:HG23	5:P:178:ARG:HB2	1.92	0.50
2:C:502:PRO:HB2	2:C:509:ALA:HB3	1.93	0.50
3:D:561:GLY:HA3	5:F:132:ARG:HD3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:828:LYS:HG2	3:D:829:VAL:O	2.12	0.50
1:A:106:PRO:HG3	1:A:134:GLU:HG2	1.94	0.50
1:B:128:HIS:HE1	1:B:131:THR:HG23	1.77	0.49
3:N:647:ARG:HH11	3:N:724:GLN:HG3	1.76	0.49
5:P:89:GLY:HA3	6:J:7:DG:C6	2.47	0.49
3:N:974:ILE:HD13	3:N:991:GLN:HB3	1.94	0.49
1:A:103:ALA:HB1	1:A:107:LYS:HD3	1.94	0.49
2:C:243:ARG:NH2	6:G:9:DG:O6	2.40	0.49
2:C:712:ALA:HB3	2:C:821:GLU:HG3	1.94	0.49
3:D:266:GLU:HG3	3:D:314:PRO:HB3	1.93	0.49
1:K:56:VAL:HG23	1:K:167:VAL:HG21	1.93	0.49
2:M:385:PHE:O	2:M:389:SER:HB3	2.12	0.49
3:N:71:LYS:NZ	3:N:74:GLU:OE2	2.36	0.49
3:N:1094:LEU:HD22	3:N:1260:ILE:HG12	1.94	0.49
6:J:10:DA:H2"	6:J:11:DG:H8	1.76	0.49
2:C:557:ARG:HG3	2:C:844:GLY:HA3	1.94	0.49
2:M:808:ARG:NH2	5:P:305:GLU:OE2	2.46	0.49
2:M:1116:ALA:HB2	3:N:88:TYR:HB3	1.95	0.49
3:D:936:TYR:O	3:D:940:THR:OG1	2.30	0.49
3:N:438:ASP:OD2	3:N:441:ARG:NH2	2.45	0.49
3:D:1099:VAL:O	3:D:1103:HIS:HB3	2.12	0.49
2:C:711:GLU:HG2	2:C:822:VAL:HG23	1.94	0.49
2:M:1063:ARG:HG3	5:P:341:PRO:HG3	1.95	0.49
6:G:18:DC:H2"	6:G:19:DG:C8	2.48	0.49
1:L:216:GLU:OE1	1:L:219:ARG:NH2	2.43	0.49
2:M:12:VAL:HG11	2:M:472:ARG:HD3	1.93	0.49
2:M:775:ARG:HD3	2:M:782:ALA:HB2	1.95	0.49
3:N:936:TYR:O	3:N:940:THR:OG1	2.31	0.49
3:N:1380:GLU:HB2	3:N:1420:LEU:HD22	1.95	0.49
3:D:760:ARG:HH22	4:E:62:THR:HG1	1.59	0.49
3:D:1094:LEU:HD22	3:D:1260:ILE:HG12	1.94	0.49
1:K:152:PRO:HD2	1:K:155:LYS:HB2	1.94	0.49
3:N:206:ARG:HD3	3:N:394:LEU:HB2	1.94	0.49
3:N:355:VAL:HG11	3:N:385:VAL:HG21	1.95	0.49
2:C:146:VAL:HG11	2:C:306:THR:HG22	1.95	0.48
3:D:1089:ALA:HA	7:H:14:DG:C8	2.47	0.48
3:D:1137:ARG:O	3:D:1141:GLU:HG3	2.13	0.48
2:M:690:ILE:HG22	2:M:869:VAL:HG22	1.94	0.48
3:N:26:VAL:HG11	3:N:44:LEU:HD23	1.95	0.48
5:P:84:TYR:O	5:P:88:ILE:HG12	2.13	0.48
2:C:212:GLY:HA2	2:C:218:VAL:HG21	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:537:LYS:HD3	2:C:583:LEU:HD11	1.94	0.48
5:F:370:LYS:HB3	5:F:376:ILE:HG13	1.94	0.48
1:L:80:LEU:HD21	3:N:842:VAL:HG12	1.96	0.48
2:M:425:PHE:HE1	3:N:1086:LEU:HD12	1.78	0.48
2:M:497:ALA:HB3	2:M:532:MET:HG3	1.93	0.48
3:N:954:ALA:HB3	3:N:1062:ARG:HD2	1.95	0.48
3:N:1350:GLU:O	3:N:1354:LYS:HG3	2.13	0.48
4:O:45:ARG:NH1	4:O:56:ASP:OD2	2.46	0.48
5:P:401:GLU:HG2	5:P:402:ASN:N	2.28	0.48
1:A:20:TYR:OH	1:A:198:ARG:HD2	2.13	0.48
2:C:755:LEU:HD22	2:C:825:VAL:HG11	1.95	0.48
3:D:777:PRO:HG2	3:D:912:LYS:HG3	1.94	0.48
4:E:49:GLN:NE2	4:E:50:THR:O	2.46	0.48
3:N:1068:LEU:O	3:N:1072:ILE:HG12	2.14	0.48
2:C:194:VAL:HG22	2:C:221:LEU:HD23	1.95	0.48
3:D:224:ARG:NE	3:D:254:GLU:OE2	2.33	0.48
3:D:544:TYR:O	3:D:548:ILE:HG12	2.13	0.48
2:M:91:GLN:HB2	2:M:117:HIS:HB3	1.95	0.48
3:N:939:PHE:O	3:N:943:THR:HG23	2.14	0.48
3:D:654:LYS:O	3:D:658:LEU:HG	2.14	0.48
5:F:361:LEU:HB3	5:F:365:GLU:HG3	1.96	0.48
3:N:245:LEU:HD13	3:N:249:TYR:HB3	1.96	0.48
3:N:520:LEU:HD12	3:N:521:PRO:HD2	1.96	0.48
3:N:703:ASN:HB2	3:N:713:ILE:HG12	1.96	0.48
5:P:358:LEU:HD21	5:P:370:LYS:HG3	1.96	0.48
2:C:124:ASP:HB3	2:C:592:LEU:HD12	1.96	0.48
3:N:114:THR:HG23	3:N:495:ARG:HG2	1.96	0.48
2:C:218:VAL:O	2:C:222:MET:HG2	2.14	0.48
3:D:897:TRP:CH2	3:D:902:LEU:HD22	2.49	0.48
5:F:387:GLY:HA2	5:F:397:ILE:HG13	1.95	0.48
2:M:805:ARG:HE	2:M:807:ARG:HD3	1.79	0.48
2:M:1009:SER:HB3	3:N:651:GLU:O	2.14	0.48
3:N:1497:GLU:O	3:N:1501:GLU:HG2	2.14	0.48
3:D:134:VAL:HG12	3:D:454:ALA:HB2	1.96	0.48
3:D:808:THR:HB	3:D:810:GLU:HG2	1.95	0.48
5:F:193:ARG:HB3	6:G:7:DG:H5"	1.94	0.48
1:L:150:TYR:CE2	1:L:170:VAL:HG22	2.49	0.48
2:M:740:GLU:HB3	2:M:805:ARG:NH1	2.29	0.47
3:N:48:ARG:NE	3:N:76:CYS:O	2.46	0.47
3:N:1130:ARG:HD2	3:N:1130:ARG:HA	1.56	0.47
1:B:106:PRO:HA	1:B:132:LEU:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:114:THR:HG23	3:D:495:ARG:HG2	1.96	0.47
3:D:128:TYR:OH	3:D:579:ASP:OD2	2.29	0.47
3:D:787:LEU:HD21	3:D:947:ILE:HG21	1.95	0.47
3:D:801:GLY:HA2	3:D:821:VAL:HG22	1.95	0.47
2:M:68:PHE:HA	2:M:98:LEU:HD23	1.96	0.47
2:M:189:ARG:NH1	2:M:242:LEU:HA	2.28	0.47
2:M:922:PHE:HB2	2:M:967:PHE:CD2	2.49	0.47
3:N:208:PRO:HG2	3:N:353:VAL:HG21	1.94	0.47
5:P:321:ILE:HG13	5:P:332:PHE:HE2	1.78	0.47
5:P:397:ILE:HA	5:P:400:ILE:HG22	1.95	0.47
1:A:112:ARG:HB3	1:A:125:PRO:HB3	1.95	0.47
2:C:221:LEU:HD11	2:C:307:LEU:HD21	1.95	0.47
2:M:643:VAL:HG11	2:M:655:LEU:HD23	1.95	0.47
2:C:597:ALA:HB2	2:C:655:LEU:HD21	1.97	0.47
3:D:800:LYS:HB3	3:D:822:ALA:H	1.78	0.47
3:D:1094:LEU:O	3:D:1098:LEU:HG	2.13	0.47
1:K:150:TYR:CE2	1:K:152:PRO:HG3	2.50	0.47
2:M:124:ASP:OD2	2:M:407:LYS:NZ	2.39	0.47
3:N:1336:LEU:HB2	3:N:1344:VAL:HG21	1.96	0.47
2:C:805:ARG:HE	2:C:807:ARG:HD3	1.79	0.47
3:D:1461:GLY:O	3:D:1465:ASN:ND2	2.48	0.47
3:N:45:PHE:HZ	3:N:541:ASN:HD21	1.62	0.47
3:N:215:TYR:HE1	3:N:381:ALA:H	1.63	0.47
1:A:31:GLY:N	1:A:193:ASP:OD2	2.47	0.47
1:B:185:ARG:HB3	1:B:190:THR:HG23	1.97	0.47
2:C:1000:MET:O	2:C:1004:LYS:HG2	2.14	0.47
2:M:39:ARG:NH1	2:M:71:TYR:O	2.35	0.47
3:N:1101:VAL:O	3:N:1374:GLN:HG2	2.14	0.47
2:C:118:ILE:HD11	2:C:344:PHE:CE1	2.50	0.47
3:D:270:LEU:HD13	3:D:304:LEU:HD13	1.97	0.47
5:F:321:ILE:HB	5:F:327:SER:OG	2.15	0.47
2:M:541:SER:O	2:M:545:ASN:ND2	2.43	0.47
3:N:1288:GLU:HG3	3:N:1289:LYS:HG3	1.96	0.47
4:O:41:GLU:HB2	4:O:44:GLU:HG3	1.97	0.47
2:C:1100:GLN:HG3	3:D:9:ARG:HH21	1.78	0.47
2:M:195:LEU:O	2:M:199:VAL:HG23	2.15	0.47
2:M:214:TYR:HE2	2:M:312:ALA:HA	1.80	0.47
2:M:1019:GLN:HG3	2:M:1058:ASP:HB3	1.97	0.47
5:F:129:GLU:HB3	5:F:151:LEU:HD21	1.97	0.47
1:K:175:ARG:HE	1:K:202:ASP:HB3	1.80	0.47
2:M:146:VAL:HG22	2:M:162:ILE:HG12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:LEU:HD22	1:B:215:VAL:HG13	1.97	0.47
2:C:719:PRO:HB3	2:C:820:ARG:NE	2.30	0.47
3:D:236:TYR:CZ	3:D:242:LEU:HD12	2.50	0.47
3:D:1147:ARG:HD3	3:D:1188:VAL:HG11	1.96	0.47
2:M:35:PRO:HG2	2:M:38:LYS:HB2	1.96	0.47
3:D:1068:LEU:O	3:D:1072:ILE:HG12	2.15	0.46
4:E:33:HIS:NE2	4:E:89:MET:HB3	2.30	0.46
1:K:156:HIS:NE2	1:K:167:VAL:O	2.29	0.46
5:P:383:LEU:HA	5:P:386:VAL:HG12	1.98	0.46
7:H:14:DG:H2'	7:H:15:DC:H6	1.80	0.46
2:C:835:VAL:HG12	3:D:632:VAL:HG21	1.97	0.46
2:M:141:HIS:HE1	2:M:332:ARG:HH11	1.63	0.46
2:M:605:LYS:HB2	2:M:612:VAL:HB	1.95	0.46
2:C:177:GLU:HG3	2:C:178:PRO:HD2	1.98	0.46
3:N:1190:SER:OG	3:N:1369:GLU:OE1	2.27	0.46
5:P:152:ASP:O	5:P:156:VAL:HG13	2.15	0.46
3:D:411:THR:O	5:F:178:ARG:NH1	2.42	0.46
2:M:682:TYR:HA	3:N:633:VAL:HG11	1.98	0.46
3:N:100:ALA:HA	3:N:513:ILE:HG13	1.97	0.46
3:N:570:GLU:OE2	5:P:214:GLN:NE2	2.44	0.46
3:N:1144:LEU:O	3:N:1147:ARG:HG3	2.16	0.46
2:C:48:PHE:CD1	2:C:348:LEU:HD21	2.51	0.46
2:C:648:ARG:HH11	2:C:648:ARG:HB3	1.80	0.46
3:D:214:GLU:OE1	3:D:342:PRO:HB3	2.16	0.46
2:M:1001:VAL:HG22	3:N:630:VAL:HB	1.96	0.46
3:N:643:GLY:HA3	3:N:727:GLN:HB2	1.96	0.46
3:D:573:MET:SD	5:F:210:LEU:HB3	2.54	0.46
1:L:124:ASN:OD1	1:L:124:ASN:N	2.48	0.46
1:L:172:SER:OG	1:L:174:VAL:O	2.33	0.46
2:M:1019:GLN:HE22	3:N:617:ASN:HB3	1.81	0.46
3:N:1089:ALA:HA	7:Q:14:DG:C8	2.50	0.46
5:P:412:GLU:HA	5:P:415:THR:HG22	1.97	0.46
3:N:5:VAL:O	3:N:1470:ARG:NH2	2.48	0.46
3:N:14:SER:HB3	3:N:511:TRP:CE2	2.51	0.46
3:N:474:GLU:HG3	3:N:496:LEU:HD11	1.97	0.46
3:N:804:LEU:O	3:N:827:ILE:HG13	2.16	0.46
3:N:1310:ARG:HB2	3:N:1327:ARG:HB2	1.97	0.46
3:N:1458:GLU:HB2	3:N:1460:ILE:HD13	1.97	0.46
5:P:93:LEU:HD21	5:P:193:ARG:HD2	1.96	0.46
1:A:198:ARG:HD3	2:C:934:PHE:CZ	2.50	0.46
2:C:1070:ILE:CG2	3:D:655:PRO:HB2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:185:LYS:HA	2:M:189:ARG:O	2.16	0.46
2:M:598:GLU:O	2:M:651:LYS:HG3	2.15	0.46
2:M:1097:LEU:HD11	3:N:103:TRP:HZ3	1.81	0.46
7:H:6:DA:H2'	7:H:7:DT:H71	1.98	0.46
1:A:24:VAL:HA	1:A:195:LEU:O	2.16	0.46
2:C:535:SER:O	2:C:538:GLN:HG2	2.16	0.46
3:D:231:VAL:O	3:D:236:TYR:OH	2.34	0.46
2:M:1016:ILE:O	3:N:87:ARG:NH1	2.48	0.46
3:N:192:ALA:HB3	3:N:195:VAL:HB	1.98	0.46
3:N:614:PHE:HA	3:N:618:LEU:HD12	1.96	0.46
2:C:607:ASP:HB2	2:C:610:ARG:NH1	2.31	0.46
2:C:1058:ASP:OD2	3:D:621:LYS:HE3	2.16	0.46
3:D:361:VAL:O	3:D:382:GLU:HA	2.15	0.46
3:D:1381:VAL:HG21	3:D:1389:LEU:HD23	1.96	0.46
1:K:104:GLU:HG2	1:K:137:ARG:HG2	1.98	0.46
2:C:637:LEU:HA	2:C:659:PRO:HG3	1.98	0.45
2:C:708:TYR:HB3	2:C:790:LEU:HD21	1.98	0.45
2:C:853:LEU:HB2	2:C:858:MET:HE1	1.98	0.45
3:D:895:VAL:O	3:D:899:LEU:HG	2.16	0.45
3:D:996:TRP:CD2	3:D:1056:PRO:HG3	2.51	0.45
2:M:580:MET:HB3	2:M:584:GLU:CD	2.35	0.45
2:M:940:GLU:HG2	2:M:973:VAL:HG21	1.98	0.45
3:N:1094:LEU:O	3:N:1098:LEU:HG	2.16	0.45
2:C:670:GLN:OE1	2:C:700:TYR:N	2.48	0.45
2:C:983:ILE:HG21	2:C:987:ILE:HD11	1.97	0.45
5:F:120:THR:HG22	5:F:122:LEU:HD13	1.96	0.45
5:F:321:ILE:HB	5:F:327:SER:HG	1.82	0.45
1:L:189:ARG:HH21	1:L:192:LEU:HD21	1.81	0.45
2:M:237:ARG:O	2:M:241:LEU:HG	2.17	0.45
2:M:709:GLU:HG3	2:M:824:ARG:HG2	1.98	0.45
3:N:1496:GLU:O	3:N:1499:ARG:HG2	2.16	0.45
6:G:18:DC:H2"	6:G:19:DG:H8	1.80	0.45
3:D:166:GLN:HB2	3:D:394:LEU:HD11	1.98	0.45
3:D:356:PRO:HB3	3:D:441:ARG:HA	1.97	0.45
5:F:373:LYS:HA	5:F:373:LYS:HD3	1.64	0.45
2:M:657:ASP:OD2	2:M:663:ASN:N	2.42	0.45
3:N:610:LYS:HD2	7:Q:15:DC:OP1	2.16	0.45
3:N:840:LYS:HE3	3:N:841:TYR:CZ	2.51	0.45
3:N:895:VAL:O	3:N:899:LEU:HG	2.17	0.45
3:N:1383:ASP:HB3	3:N:1416:ALA:HB3	1.99	0.45
3:D:200:ASP:N	3:D:200:ASP:OD1	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1377:LYS:HE3	3:D:1378:TYR:CZ	2.51	0.45
2:M:1090:LYS:HA	2:M:1090:LYS:HD3	1.78	0.45
3:N:471:GLU:H	3:N:471:GLU:HG2	1.44	0.45
1:B:153:ALA:HB1	1:B:166:PRO:HB2	1.98	0.45
2:C:251:ASP:OD1	2:C:251:ASP:N	2.39	0.45
1:K:53:VAL:HG22	1:K:144:VAL:HG22	1.98	0.45
1:L:150:TYR:HE2	1:L:170:VAL:HG22	1.80	0.45
2:M:250:ARG:CZ	2:M:250:ARG:HB3	2.45	0.45
2:M:731:GLU:HA	2:M:734:LEU:HD12	1.96	0.45
3:N:583:ASP:CG	3:N:586:ARG:HG2	2.37	0.45
1:B:150:TYR:CE1	1:B:170:VAL:HG22	2.51	0.45
2:C:631:SER:HB3	2:C:637:LEU:HG	1.97	0.45
3:D:487:ALA:O	3:D:491:LYS:HG2	2.16	0.45
2:M:235:LEU:HD21	2:M:254:VAL:HG23	1.99	0.45
2:M:344:PHE:HD1	2:M:382:ILE:HD11	1.80	0.45
3:N:573:MET:SD	5:P:210:LEU:HB3	2.56	0.45
6:J:11:DG:H2'	6:J:12:DC:C5	2.52	0.45
1:A:11:PHE:O	1:B:228:PRO:HA	2.17	0.45
2:C:577:PRO:HB3	2:C:993:PHE:CG	2.52	0.45
3:D:1053:PHE:CZ	3:D:1072:ILE:HD12	2.52	0.45
2:M:939:ARG:H	2:M:939:ARG:HG2	1.40	0.45
3:N:62:LYS:HB3	11:N:1704:HOH:O	2.16	0.45
3:N:959:GLU:OE1	3:N:959:GLU:N	2.41	0.45
1:A:57:TYR:CG	1:A:161:ARG:HD2	2.52	0.45
3:D:1493:LYS:O	3:D:1497:GLU:HG2	2.17	0.45
3:N:1040:GLY:O	3:N:1060:SER:HB3	2.16	0.45
1:A:66:SER:HB2	1:A:75:VAL:HG21	1.99	0.45
2:C:582:GLY:N	2:C:584:GLU:OE2	2.47	0.45
1:K:58:ILE:HG12	1:K:140:MET:HB3	1.99	0.45
3:D:1042:ARG:HB3	3:D:1057:VAL:HB	1.99	0.45
2:M:3:ILE:HD13	2:M:900:ARG:HB2	1.98	0.45
7:Q:4:DG:H2'	7:Q:5:DC:C6	2.52	0.45
1:B:85:LEU:HA	1:B:124:ASN:HD21	1.82	0.44
3:D:465:LEU:HD12	3:D:513:ILE:HD13	1.98	0.44
3:D:1379:VAL:HG21	3:D:1400:VAL:HG11	1.98	0.44
1:K:32:PHE:HE1	1:L:47:SER:HG	1.64	0.44
2:M:17:PRO:HB2	2:M:20:GLU:HB3	1.99	0.44
4:O:13:VAL:HG21	4:O:19:LEU:HB2	1.98	0.44
2:C:150:PRO:HD3	2:C:322:VAL:HG11	1.98	0.44
3:D:73:CYS:HB3	3:D:76:CYS:SG	2.56	0.44
5:F:386:VAL:HG12	5:F:397:ILE:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:57:TYR:CD1	1:K:161:ARG:HD2	2.52	0.44
1:L:132:LEU:HD21	1:L:138:LEU:HB2	1.99	0.44
2:M:105:THR:HG22	2:M:107:LEU:H	1.82	0.44
2:M:1092:LEU:HD13	2:M:1099:VAL:HG21	2.00	0.44
3:N:141:ILE:HA	3:N:146:PRO:HA	1.98	0.44
2:C:351:LEU:HD12	2:C:375:SER:HA	1.99	0.44
2:C:922:PHE:HB2	2:C:967:PHE:CD2	2.53	0.44
3:D:474:GLU:HG3	3:D:496:LEU:HD11	1.99	0.44
2:M:944:LEU:HD21	2:M:963:LEU:HD23	1.99	0.44
3:N:526:PRO:HB2	3:N:528:VAL:HG13	1.98	0.44
2:C:259:GLY:HA2	2:C:263:ASP:HB2	2.00	0.44
5:F:166:LEU:HB3	5:F:170:HIS:HB2	2.00	0.44
2:M:1009:SER:O	3:N:624:ASP:HB3	2.18	0.44
3:N:352:ASN:OD1	3:N:352:ASN:N	2.50	0.44
3:N:586:ARG:HD2	3:N:586:ARG:HA	1.80	0.44
7:Q:9:DC:H2"	7:Q:10:DG:H8	1.82	0.44
1:A:57:TYR:CD1	1:A:161:ARG:HD2	2.52	0.44
1:B:91:ASN:HB3	1:B:94:LEU:HB2	2.00	0.44
2:C:436:GLY:HA2	2:C:538:GLN:O	2.18	0.44
2:C:1037:VAL:HG13	2:C:1049:LEU:HD11	1.98	0.44
3:D:711:LEU:HD13	3:D:778:LEU:HD11	2.00	0.44
2:M:880:MET:HA	3:N:1038:LEU:HD21	2.00	0.44
1:A:133:GLU:HG2	1:A:134:GLU:N	2.32	0.44
2:C:74:GLY:HA3	2:C:93:PRO:HG2	2.00	0.44
2:C:881:ASN:O	2:C:884:GLN:HG2	2.17	0.44
3:D:300:LYS:HE3	3:D:300:LYS:HB2	1.83	0.44
3:D:886:VAL:O	3:D:890:VAL:HG22	2.18	0.44
3:D:1047:LYS:HG2	3:D:1053:PHE:CE1	2.53	0.44
2:M:805:ARG:NH2	2:M:821:GLU:OE1	2.51	0.44
3:N:101:HIS:CE1	3:N:582:LEU:HD13	2.52	0.44
7:Q:5:DC:H2'	7:Q:6:DA:C8	2.52	0.44
3:D:206:ARG:HD2	3:D:206:ARG:HA	1.79	0.44
3:D:1406:ARG:O	3:D:1410:GLU:HB2	2.18	0.44
5:F:384:GLU:OE2	5:F:394:ARG:NE	2.48	0.44
3:N:15:PRO:O	3:N:19:ARG:HG3	2.18	0.44
3:N:296:GLU:HG3	3:N:297:ILE:N	2.33	0.44
2:C:1090:LYS:HD3	2:C:1090:LYS:HA	1.75	0.44
1:L:83:LYS:HE2	1:L:168:ASP:HB2	2.00	0.44
2:M:896:PHE:HB2	2:M:921:ALA:HB1	2.00	0.44
2:C:87:ASP:HA	2:C:131:GLY:HA3	2.00	0.44
3:D:214:GLU:HB3	3:D:340:THR:HB	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1130:ARG:HA	3:D:1130:ARG:HD3	1.70	0.44
5:F:392:VAL:HG23	5:F:397:ILE:HG12	2.00	0.44
2:M:191:PHE:CZ	2:M:238:LEU:HD11	2.52	0.44
3:N:1047:LYS:HG2	3:N:1053:PHE:CZ	2.53	0.44
1:A:36:LEU:HD23	1:A:36:LEU:HA	1.88	0.43
1:A:73:GLU:N	1:A:73:GLU:OE1	2.50	0.43
1:A:184:THR:O	1:A:192:LEU:HB2	2.18	0.43
2:C:13:ILE:HD13	2:C:483:VAL:HG11	2.00	0.43
2:C:684:PHE:HE1	3:D:782:SER:HG	1.65	0.43
3:D:9:ARG:HB2	3:D:1456:LYS:HG2	2.00	0.43
3:D:828:LYS:HA	3:D:833:GLU:HA	1.99	0.43
3:D:1258:ARG:NH1	3:D:1261:GLU:OE2	2.45	0.43
3:D:1289:LYS:HG2	3:D:1290:LEU:H	1.82	0.43
2:M:191:PHE:HB2	2:M:192:PRO:HD2	2.00	0.43
3:N:658:LEU:HA	3:N:661:MET:HE3	2.00	0.43
2:C:247:PRO:HA	2:C:248:PRO:HD3	1.75	0.43
4:E:66:LYS:O	4:E:70:THR:HG23	2.17	0.43
5:F:372:ARG:HG2	5:F:386:VAL:HG21	2.00	0.43
2:M:561:GLY:O	2:M:565:GLN:HG3	2.18	0.43
3:N:181:ASP:HB2	3:N:205:TYR:CD2	2.52	0.43
3:N:483:HIS:HA	3:N:484:PRO:HD3	1.89	0.43
3:N:567:ILE:HG22	3:N:571:LYS:HE3	2.00	0.43
3:N:638:LYS:HA	3:N:638:LYS:HD3	1.88	0.43
3:N:1071:PHE:O	3:N:1074:SER:OG	2.32	0.43
5:P:383:LEU:HD11	5:P:398:ARG:HD3	1.99	0.43
2:C:496:ILE:HG12	2:C:531:PHE:HB2	2.00	0.43
2:C:1110:ASP:OD2	2:C:1114:GLY:N	2.49	0.43
1:L:44:LEU:O	1:L:174:VAL:HG11	2.19	0.43
2:M:195:LEU:HG	2:M:238:LEU:HB2	2.01	0.43
3:N:783:ARG:H	3:N:783:ARG:HG2	1.32	0.43
3:N:1258:ARG:NH2	3:N:1351:GLU:HG2	2.33	0.43
3:N:1379:VAL:HG21	3:N:1400:VAL:HG11	1.99	0.43
5:P:364:ARG:O	5:P:368:VAL:HG13	2.18	0.43
2:C:6:PHE:CE1	2:C:909:ALA:HB2	2.54	0.43
2:C:944:LEU:HD21	2:C:963:LEU:HD23	2.00	0.43
3:D:959:GLU:OE1	3:D:959:GLU:N	2.50	0.43
2:M:374:ASN:OD1	5:P:276:ARG:HD3	2.17	0.43
2:M:677:MET:SD	2:M:987:ILE:HD13	2.59	0.43
3:N:214:GLU:OE1	3:N:342:PRO:HB3	2.19	0.43
3:N:881:LEU:O	3:N:885:ILE:HG13	2.18	0.43
3:N:1236:LEU:HD22	3:N:1355:VAL:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:215:TYR:HE2	3:D:381:ALA:H	1.66	0.43
3:D:218:LYS:HG2	3:D:338:GLU:HG2	2.00	0.43
3:D:638:LYS:HA	3:D:638:LYS:HD3	1.82	0.43
5:P:201:LYS:NZ	5:P:244:ARG:HH21	2.17	0.43
1:B:101:LEU:HB2	1:B:114:PHE:CD1	2.53	0.43
2:C:1020:PRO:HD2	3:D:622:ARG:O	2.19	0.43
2:C:1102:LEU:HD23	2:C:1108:PRO:HA	2.00	0.43
3:D:963:TYR:CE1	3:D:1002:LYS:HD3	2.54	0.43
1:L:56:VAL:HG22	1:L:142:VAL:HG12	2.01	0.43
2:M:402:SER:HA	2:M:566:THR:HG23	2.01	0.43
2:M:1037:VAL:HG13	2:M:1049:LEU:HD11	1.99	0.43
3:N:1147:ARG:HD3	3:N:1188:VAL:HG11	2.01	0.43
3:N:1278:ASP:HA	3:N:1319:VAL:O	2.19	0.43
1:A:150:TYR:CD1	2:C:696:LYS:HG2	2.53	0.43
1:B:80:LEU:HD21	3:D:842:VAL:HG12	2.00	0.43
3:D:643:GLY:HA3	3:D:727:GLN:HB2	2.00	0.43
3:D:703:ASN:HB2	3:D:713:ILE:HG12	2.00	0.43
5:F:152:ASP:OD1	5:F:152:ASP:N	2.49	0.43
1:K:230:ALA:HA	1:L:13:VAL:O	2.18	0.43
3:N:268:ALA:HB3	3:N:284:LEU:HD12	2.00	0.43
3:N:783:ARG:HB3	3:N:1028:ALA:O	2.18	0.43
1:A:111:ALA:HB3	1:A:125:PRO:HA	1.99	0.43
3:D:770:LEU:HA	3:D:777:PRO:HA	1.99	0.43
3:D:1047:LYS:HG2	3:D:1053:PHE:CZ	2.54	0.43
4:O:42:PRO:HA	4:O:45:ARG:HD2	2.00	0.43
2:C:358:ARG:HH22	2:C:374:ASN:HD22	1.66	0.43
3:D:274:ARG:NH1	3:D:279:VAL:HG21	2.34	0.43
3:D:574:LEU:O	3:D:578:VAL:HG23	2.18	0.43
4:E:83:ASP:OD1	4:E:83:ASP:N	2.52	0.43
5:F:279:GLN:HG3	5:F:280:GLN:N	2.34	0.43
2:M:765:SER:O	2:M:767:PRO:HD3	2.19	0.43
1:K:8:ALA:HA	1:K:9:PRO:HD3	1.85	0.43
1:L:77:GLU:O	1:L:81:ASN:ND2	2.50	0.43
1:L:174:VAL:HA	1:L:201:THR:HA	2.01	0.43
2:M:577:PRO:HB3	2:M:993:PHE:CG	2.54	0.43
2:C:588:VAL:HG13	2:C:593:ALA:HB3	2.00	0.42
2:C:905:ILE:HG23	2:C:906:PHE:CD2	2.49	0.42
3:D:1000:THR:HG23	3:D:1036:ARG:HD2	2.00	0.42
5:F:101:GLU:HG3	5:F:105:LYS:HE2	2.01	0.42
1:L:153:ALA:HA	1:L:156:HIS:NE2	2.33	0.42
2:M:367:LEU:HD13	2:M:372:LEU:HD11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1487:VAL:HG22	3:N:1491:THR:HB	2.01	0.42
5:P:404:ALA:O	5:P:408:LEU:HB2	2.18	0.42
3:D:782:SER:OG	3:D:783:ARG:HG2	2.18	0.42
2:M:462:ASP:OD1	2:M:466:PHE:N	2.49	0.42
3:N:658:LEU:HB3	3:N:670:VAL:HG13	2.02	0.42
2:C:163:ILE:HG23	2:C:171:TRP:NE1	2.34	0.42
2:C:874:LEU:HD23	3:D:1023:MET:SD	2.59	0.42
2:C:922:PHE:CE2	2:C:964:LYS:HB2	2.54	0.42
1:K:68:ILE:H	1:K:68:ILE:HG13	1.60	0.42
1:K:150:TYR:CD1	2:M:696:LYS:HG2	2.54	0.42
2:M:589:ARG:HD3	2:M:596:TYR:CE1	2.55	0.42
2:M:850:ALA:HB1	3:N:633:VAL:HG12	2.02	0.42
3:N:563:PRO:HD2	3:N:566:ILE:HD12	2.00	0.42
3:N:622:ARG:NH1	7:Q:17:DT:OP1	2.52	0.42
3:N:1461:GLY:O	3:N:1465:ASN:ND2	2.52	0.42
1:A:100:LEU:HD23	1:A:141:GLU:HG2	2.00	0.42
3:D:65:ARG:HB3	3:D:67:ARG:HG3	2.01	0.42
3:D:415:VAL:HG13	3:D:419:ASP:HB2	2.01	0.42
2:M:437:ARG:NH1	2:M:491:GLU:OE2	2.48	0.42
2:C:351:LEU:HD11	2:C:373:VAL:HG13	2.02	0.42
3:D:563:PRO:HD2	3:D:566:ILE:HD12	2.01	0.42
5:F:207:LEU:HD21	5:F:254:GLN:HB2	2.00	0.42
1:L:54:THR:HG22	1:L:156:HIS:CE1	2.54	0.42
2:M:9:ILE:HD11	2:M:500:ASN:HA	1.99	0.42
2:M:74:GLY:HA3	2:M:93:PRO:HG2	2.01	0.42
3:N:132:TYR:O	3:N:152:LEU:HA	2.20	0.42
3:N:654:LYS:O	3:N:658:LEU:HG	2.20	0.42
2:C:440:PRO:HB2	3:D:1074:SER:HB2	2.02	0.42
2:C:714:ASP:OD1	2:C:820:ARG:NE	2.52	0.42
2:C:974:LEU:HD12	2:C:974:LEU:HA	1.93	0.42
3:D:462:GLN:HB2	3:D:513:ILE:HG21	2.00	0.42
3:D:618:LEU:HD13	3:D:1467:ILE:HG23	2.00	0.42
3:D:850:LEU:HD12	3:D:884:ARG:NH2	2.34	0.42
2:M:124:ASP:HB3	2:M:592:LEU:HD12	2.02	0.42
2:M:878:SER:HA	3:N:1034:GLN:OE1	2.19	0.42
3:N:1143:GLY:O	3:N:1147:ARG:HD2	2.18	0.42
5:P:287:THR:OG1	5:P:290:GLU:HG3	2.19	0.42
1:L:115:LEU:HA	1:L:116:PRO:HD3	1.95	0.42
2:M:30:LEU:HD22	2:M:73:LEU:HD11	2.02	0.42
2:M:503:LEU:HD23	2:M:508:ILE:HA	2.00	0.42
3:N:44:LEU:O	3:N:525:ARG:NH2	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:136:ASP:HB3	3:N:453:ASP:HB3	1.99	0.42
5:P:407:LYS:HD3	5:P:407:LYS:HA	1.78	0.42
7:H:4:DG:H2'	7:H:5:DC:C6	2.54	0.42
1:A:8:ALA:HA	1:A:9:PRO:HD3	1.87	0.42
1:A:111:ALA:HB2	1:A:127:LEU:HB3	2.02	0.42
2:C:267:TYR:CE2	2:C:290:LEU:HG	2.55	0.42
3:D:45:PHE:O	3:D:86:ARG:NH2	2.53	0.42
3:D:367:ILE:HB	3:D:377:VAL:HG12	2.02	0.42
3:D:1190:SER:OG	3:D:1369:GLU:OE1	2.32	0.42
3:D:1216:SER:HB3	4:E:15:SER:HA	2.02	0.42
5:F:80:PRO:HB2	5:F:210:LEU:HD11	2.02	0.42
3:N:1331:ASP:HB3	3:N:1334:GLN:HB2	2.00	0.42
2:C:680:ASP:H	3:D:943:THR:HG22	1.85	0.42
1:K:218:LEU:HG	1:L:222:LEU:HD11	2.02	0.42
2:M:385:PHE:O	2:M:389:SER:CB	2.67	0.42
2:M:400:PRO:HB3	2:M:591:SER:HB3	2.02	0.42
2:M:468:ARG:NE	2:M:487:THR:HG23	2.34	0.42
2:C:195:LEU:HD21	2:C:237:ARG:HG3	2.01	0.42
2:C:328:LEU:HD12	2:C:433:THR:O	2.20	0.42
2:C:1057:SER:OG	2:C:1058:ASP:N	2.53	0.42
3:D:310:LEU:H	3:D:310:LEU:HD12	1.85	0.42
2:M:230:ARG:HB2	2:M:231:PRO:HD2	2.02	0.42
2:M:251:ASP:OD1	2:M:251:ASP:N	2.50	0.42
2:M:708:TYR:HB3	2:M:790:LEU:HD21	2.02	0.42
2:M:1102:LEU:HD23	2:M:1108:PRO:HA	2.02	0.42
3:N:363:ALA:HB2	3:N:381:ALA:HA	2.01	0.42
3:N:684:LYS:HD3	3:N:686:GLU:OE1	2.20	0.42
5:P:373:LYS:HA	5:P:373:LYS:HD3	1.83	0.42
1:A:79:ILE:O	1:A:83:LYS:HG3	2.20	0.41
3:D:355:VAL:HG13	3:D:359:ALA:HB3	2.02	0.41
5:F:172:ARG:O	5:F:176:ILE:HG12	2.20	0.41
1:K:183:ASP:OD1	1:K:191:ASP:HA	2.20	0.41
3:N:206:ARG:HA	3:N:206:ARG:HH11	1.85	0.41
3:N:841:TYR:HB2	3:N:864:VAL:HG22	2.02	0.41
3:N:1046:GLN:N	3:N:1046:GLN:OE1	2.53	0.41
4:E:13:VAL:HG21	4:E:19:LEU:HB2	2.02	0.41
2:M:30:LEU:HD23	2:M:30:LEU:HA	1.87	0.41
2:M:139:GLN:HB2	2:M:391:LEU:HD11	2.01	0.41
2:M:215:GLY:O	2:M:216:GLU:CB	2.69	0.41
3:N:553:ARG:HD2	3:N:570:GLU:OE2	2.20	0.41
3:N:1122:LEU:HD13	3:N:1178:ALA:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:687:ALA:HB1	2:C:850:ALA:HB2	2.02	0.41
2:C:830:LYS:HE2	2:C:830:LYS:HB3	1.80	0.41
3:D:62:LYS:HD2	3:D:75:ARG:HH12	1.84	0.41
3:D:783:ARG:HD2	3:D:1029:ARG:HG2	2.02	0.41
1:L:59:GLU:HB2	1:L:139:ASN:HB3	2.02	0.41
1:L:108:GLU:HG2	1:L:131:THR:HG22	2.02	0.41
2:M:36:PRO:HA	2:M:39:ARG:HD2	2.03	0.41
3:N:209:ARG:O	3:N:346:ARG:HD3	2.20	0.41
3:N:227:LEU:HD13	3:N:331:VAL:HG13	2.03	0.41
1:A:220:GLU:O	1:A:223:THR:HB	2.20	0.41
1:B:26:GLU:HA	1:B:27:PRO:HA	1.93	0.41
5:F:95:THR:HB	5:F:98:GLU:HG3	2.02	0.41
2:M:1054:THR:O	2:M:1059:ASP:HB3	2.20	0.41
3:N:411:THR:HB	3:N:437:VAL:H	1.85	0.41
3:N:473:LEU:HD21	3:N:495:ARG:HH21	1.85	0.41
3:N:561:GLY:HA3	5:P:132:ARG:HD3	2.02	0.41
3:N:806:PHE:CE1	3:N:827:ILE:HD11	2.55	0.41
4:O:46:PRO:HD2	4:O:63:TRP:CE2	2.56	0.41
1:A:218:LEU:HG	1:B:222:LEU:HD11	2.02	0.41
3:D:401:TYR:HB3	3:D:427:VAL:HG21	2.03	0.41
3:D:1283:ILE:H	3:D:1283:ILE:HG13	1.59	0.41
1:K:9:PRO:CB	1:K:27:PRO:HD2	2.48	0.41
1:K:103:ALA:HB1	1:K:107:LYS:HD3	2.02	0.41
2:M:163:ILE:HG23	2:M:171:TRP:NE1	2.36	0.41
2:M:1070:ILE:CG2	3:N:655:PRO:HB2	2.51	0.41
2:C:206:THR:HA	2:C:209:ARG:HG2	2.03	0.41
2:C:715:THR:HB	2:C:717:LEU:H	1.85	0.41
1:L:64:GLU:HA	1:L:165:ILE:HD13	2.01	0.41
2:M:564:MET:SD	2:M:846:LYS:HD3	2.60	0.41
2:M:734:LEU:HB3	2:M:737:LEU:HD12	2.02	0.41
7:H:12:DG:H2'	7:H:13:DA:C8	2.56	0.41
1:A:228:PRO:HB3	1:B:13:VAL:HG21	2.03	0.41
2:C:425:PHE:CE2	3:D:1079:LYS:HE3	2.55	0.41
2:C:1016:ILE:O	3:D:87:ARG:NH1	2.53	0.41
3:D:1277:ILE:HG22	3:D:1278:ASP:H	1.85	0.41
5:F:193:ARG:HB2	6:G:6:DT:H1'	2.03	0.41
2:M:154:ARG:HA	2:M:155:PRO:HD3	1.85	0.41
2:M:261:ILE:HD11	2:M:303:PHE:HZ	1.85	0.41
3:N:731:LEU:HD23	3:N:731:LEU:HA	1.92	0.41
3:N:908:LYS:HB3	3:N:908:LYS:HE2	1.82	0.41
3:N:1465:ASN:HB3	3:N:1470:ARG:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:THR:HG21	1:A:145:ASP:HB2	2.02	0.41
3:D:658:LEU:HA	3:D:661:MET:HE3	2.02	0.41
3:D:842:VAL:HG22	3:D:865:THR:HB	2.02	0.41
3:D:1098:LEU:HA	3:D:1101:VAL:HG12	2.02	0.41
2:M:860:HIS:CE1	2:M:975:TYR:HB2	2.56	0.41
3:N:101:HIS:HB3	3:N:104:PHE:HD2	1.85	0.41
3:N:539:ASP:OD2	3:N:598:ARG:NH1	2.50	0.41
3:N:540:LEU:HD23	3:N:543:LEU:HD12	2.03	0.41
3:N:1236:LEU:HD13	3:N:1259:VAL:HG21	2.02	0.41
1:A:133:GLU:HG3	2:C:645:VAL:HG21	2.03	0.41
1:A:176:ARG:HG3	1:A:177:VAL:N	2.35	0.41
2:C:210:GLU:HG2	2:C:304:LEU:HD21	2.02	0.41
2:C:563:ASN:O	2:C:566:THR:HB	2.20	0.41
2:C:1032:PHE:CZ	2:C:1036:GLU:HB3	2.56	0.41
3:D:95:LEU:HD22	3:D:574:LEU:HD21	2.03	0.41
3:D:534:ARG:HE	3:D:534:ARG:HB3	1.63	0.41
3:D:661:MET:HE3	3:D:661:MET:HB2	1.95	0.41
3:D:843:PHE:CE2	3:D:864:VAL:HG11	2.56	0.41
3:D:1465:ASN:OD1	3:D:1470:ARG:NH1	2.53	0.41
1:K:41:ARG:HA	1:K:177:VAL:HG11	2.01	0.41
3:N:134:VAL:HG23	3:N:149:LYS:HA	2.03	0.41
3:N:236:TYR:CZ	3:N:242:LEU:HD12	2.56	0.41
5:P:153:PRO:HA	5:P:156:VAL:HG22	2.01	0.41
5:P:399:GLN:O	5:P:403:LYS:HG2	2.21	0.41
7:H:11:DT:H2"	7:H:12:DG:C8	2.55	0.41
2:C:895:TYR:HB2	2:C:991:GLN:HG3	2.03	0.41
3:D:353:VAL:HG12	3:D:355:VAL:H	1.85	0.41
2:M:210:GLU:HG2	2:M:304:LEU:HD21	2.03	0.41
1:B:213:GLN:O	1:B:217:ILE:HG13	2.21	0.40
2:C:675:ALA:HB2	2:C:867:VAL:HG11	2.03	0.40
2:C:861:LEU:HD12	2:C:865:THR:HB	2.03	0.40
3:D:956:ILE:HD13	3:D:1039:CYS:O	2.21	0.40
3:D:1342:GLU:CD	3:D:1342:GLU:H	2.24	0.40
1:K:108:GLU:HG2	1:K:131:THR:HG23	2.02	0.40
2:M:28:ARG:NH1	2:M:42:VAL:HG11	2.36	0.40
2:M:195:LEU:HD21	2:M:237:ARG:HG3	2.01	0.40
2:M:328:LEU:HA	2:M:328:LEU:HD23	1.79	0.40
2:M:401:LEU:HD13	2:M:587:VAL:HG11	2.03	0.40
2:M:1110:ASP:OD2	2:M:1114:GLY:N	2.31	0.40
3:N:477:LEU:HB2	3:N:496:LEU:HD13	2.04	0.40
3:N:1453:ALA:HB3	3:N:1455:LYS:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:141:VAL:O	5:P:142:ARG:HG3	2.20	0.40
1:A:16:GLN:HB2	1:A:20:TYR:HB3	2.03	0.40
1:A:64:GLU:HG3	1:A:79:ILE:HD12	2.03	0.40
1:A:183:ASP:HA	2:C:938:LYS:HE3	2.03	0.40
2:C:740:GLU:HB3	2:C:805:ARG:NH1	2.35	0.40
2:C:1042:ALA:HA	3:D:1220:ALA:HB3	2.02	0.40
3:D:897:TRP:HA	3:D:900:ILE:HD12	2.03	0.40
3:D:1127:GLU:H	3:D:1127:GLU:CD	2.25	0.40
3:D:1491:THR:O	3:D:1495:ILE:HG13	2.20	0.40
4:E:87:LYS:HA	4:E:87:LYS:HD3	1.91	0.40
5:F:181:GLU:O	5:F:185:GLN:HG2	2.21	0.40
1:K:220:GLU:O	1:K:223:THR:HB	2.21	0.40
2:M:344:PHE:CD1	2:M:382:ILE:HD11	2.56	0.40
2:C:328:LEU:HA	2:C:328:LEU:HD23	1.83	0.40
3:D:236:TYR:HD2	3:D:322:VAL:HG21	1.86	0.40
3:D:1211:MET:HB2	3:D:1211:MET:HE3	1.98	0.40
3:N:8:VAL:HG12	3:N:1434:TRP:HZ2	1.87	0.40
3:N:633:VAL:HA	3:N:740:PHE:CZ	2.56	0.40
3:N:1488:ASP:OD1	3:N:1488:ASP:N	2.48	0.40
1:B:65:PHE:CD2	3:D:809:PRO:HB2	2.56	0.40
1:B:211:LEU:O	1:B:215:VAL:HG23	2.22	0.40
2:C:66:LEU:HD11	2:C:98:LEU:HB3	2.04	0.40
2:C:589:ARG:NH2	2:C:652:GLY:O	2.49	0.40
2:C:680:ASP:OD1	3:D:943:THR:HG21	2.22	0.40
3:D:1150:ALA:HB3	3:D:1187:PRO:HB2	2.04	0.40
3:D:1216:SER:OG	4:E:16:LYS:HG2	2.21	0.40
2:M:214:TYR:CE2	2:M:312:ALA:HA	2.55	0.40
2:M:712:ALA:HB3	2:M:821:GLU:HG3	2.02	0.40
3:N:127:LEU:HA	3:N:457:GLY:HA2	2.02	0.40
3:N:255:GLU:HA	3:N:300:LYS:HE2	2.03	0.40
3:N:1485:GLN:NE2	4:O:82:GLU:OE1	2.55	0.40
5:P:234:LYS:HB3	5:P:234:LYS:HE2	1.87	0.40
1:A:176:ARG:HG2	1:A:200:TRP:CE3	2.55	0.40
1:A:201:THR:HG22	1:A:203:GLY:H	1.85	0.40
2:C:172:ILE:HD13	2:C:184:MET:HE3	2.03	0.40
2:M:236:ILE:HG23	2:M:248:PRO:HB2	2.02	0.40
3:N:943:THR:OG1	3:N:944:THR:N	2.55	0.40
3:N:1126:ASP:OD1	3:N:1126:ASP:N	2.47	0.40
3:N:1383:ASP:HA	3:N:1384:PRO:HD3	1.93	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	227/315 (72%)	220 (97%)	7 (3%)	0	100	100
1	B	220/315 (70%)	214 (97%)	6 (3%)	0	100	100
1	K	225/315 (71%)	219 (97%)	6 (3%)	0	100	100
1	L	223/315 (71%)	219 (98%)	4 (2%)	0	100	100
2	C	1107/1119 (99%)	1082 (98%)	25 (2%)	0	100	100
2	M	1107/1119 (99%)	1077 (97%)	30 (3%)	0	100	100
3	D	1482/1524 (97%)	1447 (98%)	35 (2%)	0	100	100
3	N	1482/1524 (97%)	1446 (98%)	36 (2%)	0	100	100
4	E	92/99 (93%)	90 (98%)	2 (2%)	0	100	100
4	O	92/99 (93%)	91 (99%)	1 (1%)	0	100	100
5	F	344/443 (78%)	342 (99%)	2 (1%)	0	100	100
5	P	345/443 (78%)	334 (97%)	11 (3%)	0	100	100
All	All	6946/7630 (91%)	6781 (98%)	165 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	195/273 (71%)	185 (95%)	10 (5%)	24	57
1	B	195/273 (71%)	179 (92%)	16 (8%)	11	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	K	198/273 (72%)	182 (92%)	16 (8%)	11 39
1	L	198/273 (72%)	188 (95%)	10 (5%)	24 57
2	C	931/941 (99%)	879 (94%)	52 (6%)	21 54
2	M	927/941 (98%)	879 (95%)	48 (5%)	23 56
3	D	1241/1279 (97%)	1175 (95%)	66 (5%)	22 56
3	N	1240/1279 (97%)	1181 (95%)	59 (5%)	25 59
4	E	83/88 (94%)	79 (95%)	4 (5%)	25 59
4	O	83/88 (94%)	81 (98%)	2 (2%)	49 75
5	F	300/388 (77%)	289 (96%)	11 (4%)	34 64
5	P	291/388 (75%)	281 (97%)	10 (3%)	37 67
All	All	5882/6484 (91%)	5578 (95%)	304 (5%)	23 56

All (304) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	36	LEU
1	A	67	THR
1	A	128	HIS
1	A	148	VAL
1	A	184	THR
1	A	188	GLN
1	A	189	ARG
1	A	206	THR
1	A	229	GLN
1	B	7	LYS
1	B	10	VAL
1	B	12	THR
1	B	34	VAL
1	B	38	ASN
1	B	56	VAL
1	B	66	SER
1	B	96	THR
1	B	113	ASP
1	B	114	PHE
1	B	124	ASN
1	B	133	GLU
1	B	188	GLN

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Mol	Chain	Res	Type
1	B	190	THR
1	B	191	ASP
1	B	197	LEU
2	C	1	MET
2	C	21	ILE
2	C	133	ASP
2	C	138	SER
2	C	141	HIS
2	C	149	THR
2	C	154	ARG
2	C	177	GLU
2	C	196	LEU
2	C	218	VAL
2	C	221	LEU
2	C	251	ASP
2	C	261	ILE
2	C	321	GLU
2	C	335	THR
2	C	402	SER
2	C	422	ARG
2	C	429	ASP
2	C	434	HIS
2	C	443	THR
2	C	453	THR
2	C	460	ARG
2	C	475	VAL
2	C	480	THR
2	C	482	GLU
2	C	490	GLU
2	C	513	VAL
2	C	524	VAL
2	C	575	GLN
2	C	610	ARG
2	C	617	ASP
2	C	640	ARG
2	C	648	ARG
2	C	672	VAL
2	C	683	ASN
2	C	715	THR
2	C	764	GLU
2	C	775	ARG
2	C	805	ARG

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Mol	Chain	Res	Type
2	C	807	ARG
2	C	808	ARG
2	C	822	VAL
2	C	831	ARG
2	C	846	LYS
2	C	848	VAL
2	C	887	GLU
2	C	939	ARG
2	C	1001	VAL
2	C	1058	ASP
2	C	1076	VAL
2	C	1080	SER
2	C	1106	ASP
3	D	12	LEU
3	D	65	ARG
3	D	67	ARG
3	D	68	PHE
3	D	80	VAL
3	D	115	LEU
3	D	134	VAL
3	D	184	GLU
3	D	200	ASP
3	D	231	VAL
3	D	247	GLU
3	D	256	GLU
3	D	270	LEU
3	D	275	GLU
3	D	276	ASP
3	D	286	VAL
3	D	310	LEU
3	D	331	VAL
3	D	362	GLU
3	D	399	ARG
3	D	400	VAL
3	D	500	ARG
3	D	508	ARG
3	D	514	LEU
3	D	525	ARG
3	D	586	ARG
3	D	587	ARG
3	D	647	ARG
3	D	669	ASN

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Mol	Chain	Res	Type
3	D	680	GLN
3	D	686	GLU
3	D	687	VAL
3	D	709	HIS
3	D	717	GLN
3	D	743	ASP
3	D	754	PHE
3	D	778	LEU
3	D	783	ARG
3	D	805	GLU
3	D	808	THR
3	D	827	ILE
3	D	828	LYS
3	D	875	THR
3	D	907	GLU
3	D	940	THR
3	D	943	THR
3	D	1029	ARG
3	D	1041	LEU
3	D	1055	VAL
3	D	1062	ARG
3	D	1079	LYS
3	D	1128	VAL
3	D	1130	ARG
3	D	1152	GLU
3	D	1155	VAL
3	D	1188	VAL
3	D	1216	SER
3	D	1219	GLU
3	D	1221	VAL
3	D	1253	THR
3	D	1278	ASP
3	D	1344	VAL
3	D	1408	ILE
3	D	1422	MET
3	D	1460	ILE
3	D	1486	VAL
4	E	50	THR
4	E	74	VAL
4	E	84	ARG
4	E	90	GLU
5	F	88	ILE

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Mol	Chain	Res	Type
5	F	208	SER
5	F	218	GLN
5	F	258	ILE
5	F	279	GLN
5	F	326	ASP
5	F	327	SER
5	F	363	GLU
5	F	392	VAL
5	F	396	ARG
5	F	422	LEU
1	K	6	LEU
1	K	10	VAL
1	K	25	LEU
1	K	67	THR
1	K	68	ILE
1	K	74	ASP
1	K	80	LEU
1	K	112	ARG
1	K	160	ASP
1	K	180	GLN
1	K	189	ARG
1	K	196	THR
1	K	205	VAL
1	K	206	THR
1	K	218	LEU
1	K	219	ARG
1	L	22	GLU
1	L	34	VAL
1	L	38	ASN
1	L	54	THR
1	L	96	THR
1	L	172	SER
1	L	179	PHE
1	L	189	ARG
1	L	191	ASP
1	L	206	THR
2	M	1	MET
2	M	28	ARG
2	M	85	GLU
2	M	141	HIS
2	M	149	THR
2	M	165	LEU

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Mol	Chain	Res	Type
2	M	173	ASP
2	M	182	VAL
2	M	189	ARG
2	M	194	VAL
2	M	203	ASP
2	M	211	LEU
2	M	240	THR
2	M	254	VAL
2	M	265	ARG
2	M	340	MET
2	M	357	GLU
2	M	358	ARG
2	M	394	PHE
2	M	402	SER
2	M	429	ASP
2	M	434	HIS
2	M	442	GLU
2	M	460	ARG
2	M	482	GLU
2	M	489	THR
2	M	512	ARG
2	M	513	VAL
2	M	524	VAL
2	M	525	SER
2	M	527	GLU
2	M	557	ARG
2	M	610	ARG
2	M	617	ASP
2	M	645	VAL
2	M	698	ASP
2	M	715	THR
2	M	729	LEU
2	M	730	SER
2	M	734	LEU
2	M	735	ARG
2	M	764	GLU
2	M	808	ARG
2	M	870	ILE
2	M	887	GLU
2	M	929	ARG
2	M	939	ARG
2	M	1060	ILE

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Mol	Chain	Res	Type
3	N	53	ILE
3	N	69	GLU
3	N	81	THR
3	N	97	THR
3	N	124	GLU
3	N	142	LEU
3	N	155	ASP
3	N	176	ASP
3	N	184	GLU
3	N	199	LEU
3	N	230	TRP
3	N	247	GLU
3	N	289	THR
3	N	331	VAL
3	N	372	ASP
3	N	374	GLU
3	N	405	ASP
3	N	411	THR
3	N	415	VAL
3	N	471	GLU
3	N	500	ARG
3	N	514	LEU
3	N	525	ARG
3	N	587	ARG
3	N	601	ARG
3	N	628	ARG
3	N	666	ILE
3	N	686	GLU
3	N	747	VAL
3	N	754	PHE
3	N	783	ARG
3	N	784	ASP
3	N	785	ILE
3	N	805	GLU
3	N	808	THR
3	N	864	VAL
3	N	875	THR
3	N	904	VAL
3	N	940	THR
3	N	943	THR
3	N	971	LEU
3	N	1042	ARG

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Mol	Chain	Res	Type
3	N	1067	VAL
3	N	1079	LYS
3	N	1173	LEU
3	N	1188	VAL
3	N	1200	VAL
3	N	1221	VAL
3	N	1273	VAL
3	N	1278	ASP
3	N	1284	GLU
3	N	1305	LEU
3	N	1344	VAL
3	N	1413	THR
3	N	1433	SER
3	N	1460	ILE
3	N	1486	VAL
3	N	1487	VAL
3	N	1499	ARG
4	O	62	THR
4	O	83	ASP
5	P	218	GLN
5	P	295	MET
5	P	309	LYS
5	P	363	GLU
5	P	367	MET
5	P	372	ARG
5	P	376	ILE
5	P	393	THR
5	P	401	GLU
5	P	419	ARG

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

Mol	Chain	Res	Type
2	C	704	HIS
3	D	973	GLN
2	M	141	HIS
2	M	704	HIS
3	N	994	GLN

5.3.3 RNA (i)

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

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 7 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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	229/315 (72%)	0.39	10 (4%) 34 35	63, 82, 107, 131	0
1	B	222/315 (70%)	0.55	16 (7%) 15 16	66, 96, 127, 148	0
1	K	227/315 (72%)	0.55	20 (8%) 10 10	70, 92, 113, 130	0
1	L	225/315 (71%)	0.47	18 (8%) 12 12	68, 99, 133, 152	0
2	C	1111/1119 (99%)	0.17	5 (0%) 91 91	46, 80, 132, 163	0
2	M	1111/1119 (99%)	0.28	20 (1%) 68 67	51, 100, 161, 179	0
3	D	1486/1524 (97%)	0.32	53 (3%) 42 41	48, 83, 143, 186	1 (0%)
3	N	1486/1524 (97%)	0.34	62 (4%) 36 36	52, 90, 142, 196	1 (0%)
4	E	94/99 (94%)	0.23	0 100 100	63, 85, 122, 130	0
4	O	94/99 (94%)	0.14	2 (2%) 63 63	71, 100, 137, 144	0
5	F	346/443 (78%)	0.35	16 (4%) 32 33	58, 91, 135, 158	0
5	P	347/443 (78%)	0.53	26 (7%) 14 14	70, 108, 173, 191	0
6	G	25/27 (92%)	-0.08	0 100 100	87, 128, 187, 196	0
6	J	25/27 (92%)	0.13	0 100 100	90, 134, 190, 196	0
7	H	17/19 (89%)	0.04	0 100 100	77, 110, 182, 190	0
7	Q	17/19 (89%)	0.04	0 100 100	93, 122, 186, 189	0
8	I	2/2 (100%)	0.75	0 100 100	79, 79, 79, 85	2 (100%)
8	R	2/2 (100%)	0.30	0 100 100	88, 88, 88, 93	2 (100%)
All	All	7066/7726 (91%)	0.32	248 (3%) 44 43	46, 91, 148, 196	6 (0%)

All (248) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	P	392	VAL	8.5
1	B	138	LEU	5.2
5	P	391	GLY	5.1

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Mol	Chain	Res	Type	RSRZ
3	N	394	LEU	4.8
5	P	389	PHE	4.4
3	N	191	LEU	4.3
3	N	409	VAL	4.2
3	N	177	ALA	4.1
5	F	141	VAL	4.0
3	N	410	SER	4.0
3	N	367	ILE	4.0
3	D	367	ILE	3.9
1	K	197	LEU	3.9
5	P	390	PHE	3.9
3	D	350	HIS	3.9
3	D	839	LEU	3.8
3	N	350	HIS	3.8
3	N	209	ARG	3.8
3	N	305	ALA	3.7
5	F	229	TYR	3.7
3	N	352	ASN	3.6
3	N	437	VAL	3.6
2	M	594	ALA	3.6
3	N	393	ILE	3.6
3	D	409	VAL	3.6
2	M	200	LEU	3.5
1	K	178	ALA	3.5
5	P	229	TYR	3.5
3	D	335	LEU	3.5
3	D	161	LEU	3.4
1	K	87	VAL	3.4
3	D	393	ILE	3.4
3	D	1319	VAL	3.4
3	N	269	PHE	3.4
1	L	138	LEU	3.4
3	D	223	LEU	3.3
5	P	239	ALA	3.3
1	K	174	VAL	3.3
2	M	593	ALA	3.3
3	N	432	TYR	3.3
3	N	407	VAL	3.3
3	D	321	GLN	3.3
3	N	415	VAL	3.2
1	L	165	ILE	3.2
3	N	211	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
2	M	146	VAL	3.1
5	F	163	LEU	3.1
3	N	304	LEU	3.1
5	P	393	THR	3.1
3	N	353	VAL	3.1
1	K	169	ALA	3.1
1	B	165	ILE	3.1
2	M	311	PHE	3.1
3	N	270	LEU	3.1
3	D	203	ALA	3.1
1	K	130	ALA	3.0
3	N	371	ILE	3.0
3	D	322	VAL	3.0
1	K	199	ILE	3.0
5	F	138	SER	3.0
1	K	201	THR	3.0
2	M	221	LEU	3.0
3	D	337	LEU	3.0
1	B	129	ILE	3.0
1	L	211	LEU	3.0
2	M	934	PHE	3.0
3	D	355	VAL	2.9
3	D	177	ALA	2.9
3	D	388	HIS	2.9
5	F	142	ARG	2.9
3	N	566	ILE	2.9
5	P	163	LEU	2.9
1	K	23	PHE	2.9
3	N	212	ARG	2.8
3	N	387	LEU	2.8
1	L	82	LEU	2.8
5	P	191	ASN	2.8
3	N	135	LEU	2.8
5	P	173	TYR	2.8
3	N	242	LEU	2.8
3	D	371	ILE	2.8
3	N	208	PRO	2.8
3	D	165	LYS	2.8
5	P	138	SER	2.7
3	D	352	ASN	2.7
4	O	89	MET	2.7
1	B	218	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
5	P	175	HIS	2.7
3	D	26	VAL	2.7
5	F	145	PRO	2.7
1	L	56	VAL	2.7
5	P	140	ARG	2.7
3	D	1297	GLU	2.6
5	F	140	ARG	2.6
3	N	290	PRO	2.6
5	F	175	HIS	2.6
3	D	205	TYR	2.6
3	N	307	ALA	2.6
1	K	21	GLY	2.6
3	D	197	SER	2.6
3	N	435	VAL	2.6
1	K	211	LEU	2.6
3	N	355	VAL	2.6
1	K	85	LEU	2.6
3	D	49	ILE	2.6
1	A	197	LEU	2.6
2	C	365	ASP	2.6
3	N	434	ARG	2.6
1	L	65	PHE	2.6
3	N	396	VAL	2.6
3	N	236	TYR	2.5
3	N	421	LEU	2.5
3	N	455	ARG	2.5
2	M	534	VAL	2.5
1	B	89	PHE	2.5
1	K	129	ILE	2.5
2	C	629	TYR	2.5
1	L	175	ARG	2.5
3	D	428	LYS	2.5
1	K	24	VAL	2.5
1	K	111	ALA	2.5
2	M	608	GLY	2.5
3	N	446	VAL	2.5
3	N	1017	PHE	2.5
1	A	44	LEU	2.5
3	N	858	VAL	2.5
1	B	164	ALA	2.5
3	N	165	LYS	2.5
5	P	88	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
3	D	270	LEU	2.4
3	N	213	VAL	2.4
5	P	217	ASN	2.4
1	K	225	PHE	2.4
5	P	397	ILE	2.4
1	L	150	TYR	2.4
2	C	226	VAL	2.4
3	D	283	PHE	2.4
1	A	142	VAL	2.4
3	N	317	VAL	2.4
2	M	461	VAL	2.4
1	B	82	LEU	2.4
3	N	161	LEU	2.4
3	D	144	GLY	2.4
3	N	368	VAL	2.4
1	L	218	LEU	2.4
3	N	339	TRP	2.3
3	D	384	VAL	2.3
5	P	122	LEU	2.3
5	F	230	LYS	2.3
1	L	120	VAL	2.3
1	K	99	LEU	2.3
1	L	109	VAL	2.3
5	P	386	VAL	2.3
3	D	1279	GLY	2.3
1	L	102	LYS	2.3
3	D	345	TYR	2.3
1	L	114	PHE	2.3
5	F	235	PHE	2.3
2	M	655	LEU	2.3
3	D	566	ILE	2.3
1	A	199	ILE	2.3
3	D	397	LYS	2.3
3	D	272	LEU	2.3
3	N	261	LEU	2.3
5	F	151	LEU	2.3
3	D	269	PHE	2.3
3	D	305	ALA	2.3
3	N	388	HIS	2.3
1	K	138	LEU	2.2
3	D	268	ALA	2.2
2	M	344	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	175	ARG	2.2
2	M	44	ILE	2.2
3	D	202	VAL	2.2
3	D	411	THR	2.2
3	D	491	LYS	2.2
3	N	237	LYS	2.2
3	D	333	LEU	2.2
1	B	23	PHE	2.2
3	D	470	LEU	2.2
1	A	194	LYS	2.2
5	P	141	VAL	2.2
4	O	68	LEU	2.2
3	D	353	VAL	2.2
5	P	242	TRP	2.2
3	N	397	LYS	2.2
1	B	85	LEU	2.2
1	A	211	LEU	2.1
1	K	44	LEU	2.1
2	M	174	LEU	2.1
5	P	192	LEU	2.1
2	C	219	GLN	2.1
1	L	53	VAL	2.1
2	M	252	LYS	2.1
5	F	220	LEU	2.1
5	P	174	LEU	2.1
1	L	171	PHE	2.1
3	N	153	LEU	2.1
3	N	1313	VAL	2.1
5	P	127	ILE	2.1
2	M	222	MET	2.1
1	A	20	TYR	2.1
1	B	53	VAL	2.1
3	N	199	LEU	2.1
3	D	212	ARG	2.1
3	N	406	ASP	2.1
1	A	99	LEU	2.1
1	L	25	LEU	2.1
1	L	170	VAL	2.1
3	N	30	GLU	2.1
2	M	625	LEU	2.1
5	F	172	ARG	2.1
1	B	56	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	L	141	GLU	2.1
1	B	158	ILE	2.1
3	D	422	ALA	2.1
3	D	354	VAL	2.1
3	N	1319	VAL	2.1
5	F	105	LYS	2.1
3	D	387	LEU	2.1
1	B	114	PHE	2.1
3	D	390	PRO	2.1
3	N	268	ALA	2.1
5	P	325	LYS	2.1
3	D	241	ILE	2.1
1	A	87	VAL	2.1
3	N	26	VAL	2.1
3	N	202	VAL	2.1
2	M	246	ASP	2.1
3	N	292	VAL	2.0
3	N	422	ALA	2.0
3	D	343	LYS	2.0
1	A	144	VAL	2.0
2	M	188	LYS	2.0
1	B	140	MET	2.0
3	N	347	VAL	2.0
3	D	496	LEU	2.0
5	P	243	ILE	2.0
2	M	400	PRO	2.0
3	D	831	GLY	2.0
3	N	620	GLY	2.0
5	F	217	ASN	2.0
5	P	387	GLY	2.0
1	B	58	ILE	2.0
1	K	198	ARG	2.0
5	F	196	VAL	2.0
2	C	968	LEU	2.0
3	D	43	GLY	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 monosaccharides 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, 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	B-factors(Å^2)	Q<0.9
10	MG	L	401	1/1	0.77	0.17	77,77,77,77	0
9	ZN	N	1601	1/1	0.95	0.24	93,93,93,93	0
10	MG	N	1603	1/1	0.98	0.23	61,61,61,61	0
10	MG	D	2003	1/1	0.99	0.24	54,54,54,54	0
9	ZN	D	2001	1/1	0.99	0.23	78,78,78,78	0
9	ZN	N	1602	1/1	0.99	0.15	129,129,129,129	0
9	ZN	D	2002	1/1	1.00	0.17	95,95,95,95	0

6.5 Other polymers (i)

There are no such residues in this entry.