



# Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 07:55 pm BST

PDB ID : 1L9U  
Title : THERMUS AQUATICUS RNA POLYMERASE HOLOENZYME AT 4 Å  
RESOLUTION  
Authors : Murakami, K.S.; Masuda, S.; Darst, S.A.  
Deposited on : 2002-03-26  
Resolution : 4.00 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

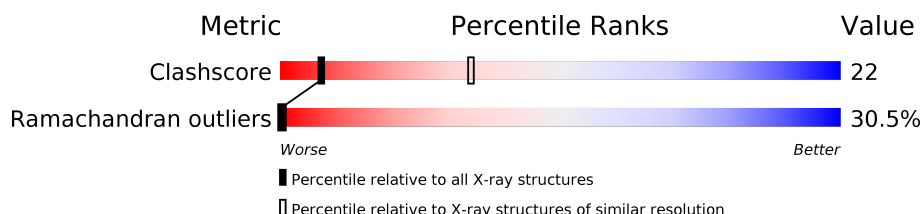
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 4.00 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))
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	314	
1	B	314	
1	J	314	
1	K	314	
2	C	1118	
2	L	1118	
3	D	1524	
3	M	1524	
4	E	99	

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Mol	Chain	Length	Quality of chain
4	N	99	<div><div></div><div>47%44%7%</div></div>
5	H	332	<div><div></div><div>75%21%. .</div></div>
5	Q	332	<div><div></div><div>75%21%. .</div></div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 18756 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 RNA POLYMERASE, ALPHA SUBUNIT.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	0	0	0
			672	448	224			
1	B	220	Total	C	N	0	0	0
			660	440	220			
1	J	224	Total	C	N	0	0	0
			672	448	224			
1	K	220	Total	C	N	0	0	0
			660	440	220			

- Molecule 2 is a protein called RNA POLYMERASE, BETA SUBUNIT.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	1084	Total	C	N	0	0	0
			3252	2168	1084			
2	L	1084	Total	C	N	0	0	0
			3252	2168	1084			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	GLU	DELETION	UNP Q9KWU7
L	?	-	GLU	DELETION	UNP Q9KWU7

- Molecule 3 is a protein called RNA POLYMERASE, BETA-PRIME SUBUNIT.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	D	1183	Total	C	N	0	0	0
			3549	2366	1183			
3	M	1183	Total	C	N	0	0	0
			3549	2366	1183			

- Molecule 4 is a protein called RNA POLYMERASE, OMEGA SUBUNIT.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	E	92	Total	C	N	0	0	0
			276	184	92			
4	N	92	Total	C	N	0	0	0
			276	184	92			

- Molecule 5 is a protein called SIGMA FACTOR SIGA.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
5	H	322	Total	C	N	0	0	0
			966	644	322			
5	Q	322	Total	C	N	0	0	0
			966	644	322			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	?	-	ILE	DELETION	UNP Q9EZJ8
H	?	-	GLN	DELETION	UNP Q9EZJ8
H	?	-	LYS	DELETION	UNP Q9EZJ8
H	?	-	ILE	DELETION	UNP Q9EZJ8
H	?	-	PRO	DELETION	UNP Q9EZJ8
H	?	-	GLY	DELETION	UNP Q9EZJ8
H	?	-	LEU	DELETION	UNP Q9EZJ8
H	?	-	LYS	DELETION	UNP Q9EZJ8
H	?	-	GLU	DELETION	UNP Q9EZJ8
H	?	-	LYS	DELETION	UNP Q9EZJ8
H	?	-	PRO	DELETION	UNP Q9EZJ8
H	?	-	ASP	DELETION	UNP Q9EZJ8
H	?	-	PRO	DELETION	UNP Q9EZJ8
H	?	-	LYS	DELETION	UNP Q9EZJ8
H	?	-	THR	DELETION	UNP Q9EZJ8
Q	?	-	ILE	DELETION	UNP Q9EZJ8
Q	?	-	GLN	DELETION	UNP Q9EZJ8
Q	?	-	LYS	DELETION	UNP Q9EZJ8
Q	?	-	ILE	DELETION	UNP Q9EZJ8
Q	?	-	PRO	DELETION	UNP Q9EZJ8
Q	?	-	GLY	DELETION	UNP Q9EZJ8
Q	?	-	LEU	DELETION	UNP Q9EZJ8
Q	?	-	LYS	DELETION	UNP Q9EZJ8
Q	?	-	GLU	DELETION	UNP Q9EZJ8
Q	?	-	LYS	DELETION	UNP Q9EZJ8
Q	?	-	PRO	DELETION	UNP Q9EZJ8
Q	?	-	ASP	DELETION	UNP Q9EZJ8

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	?	-	PRO	DELETION	UNP Q9EZJ8
Q	?	-	LYS	DELETION	UNP Q9EZJ8
Q	?	-	THR	DELETION	UNP Q9EZJ8

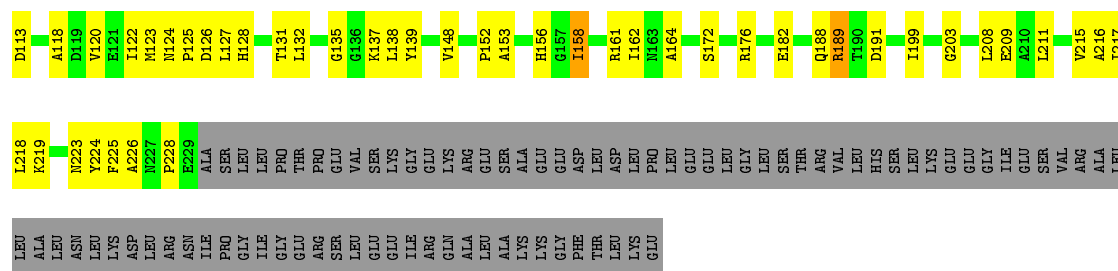
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	Total Mg 1 1	0	0
6	M	1	Total Mg 1 1	0	0

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

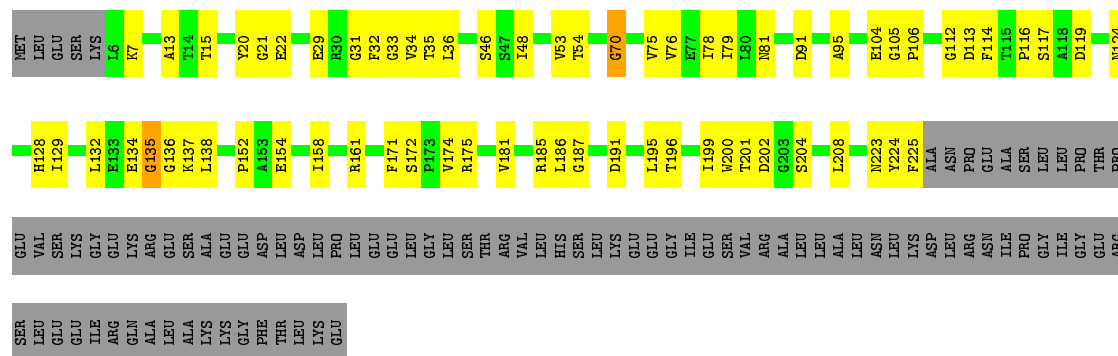
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	D	2	Total Zn 2 2	0	0
7	M	2	Total Zn 2 2	0	0





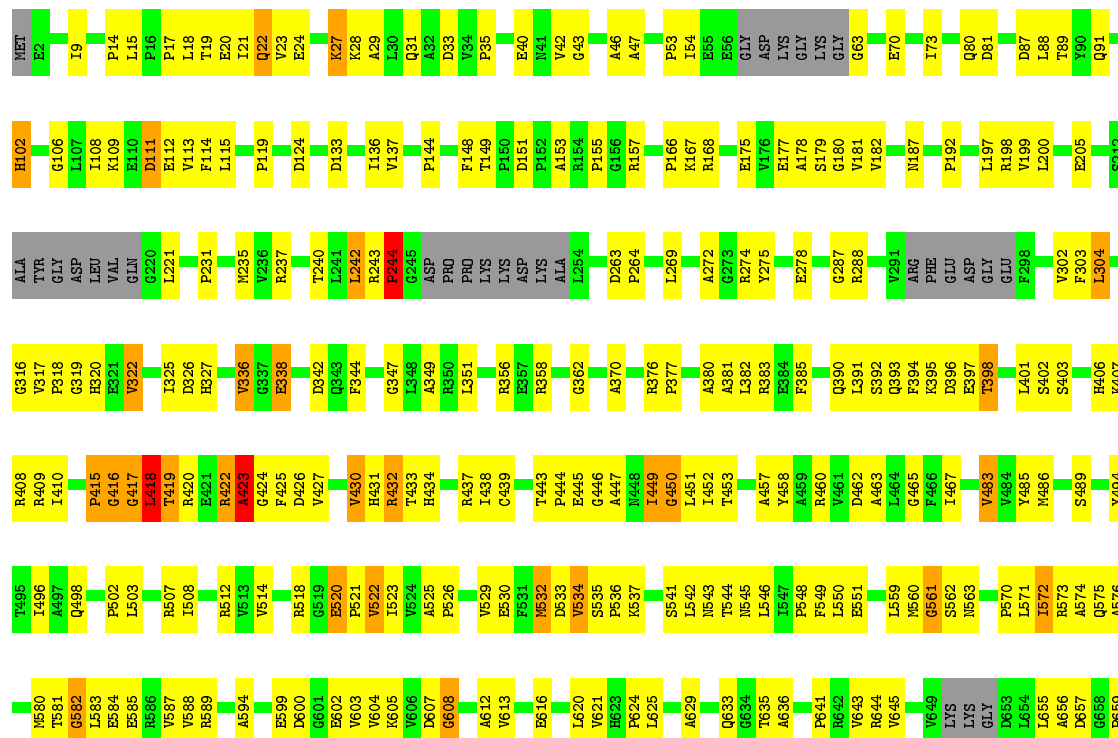
• Molecule 1: RNA POLYMERASE, ALPHA SUBUNIT

Chain K: 49% 21% 30%

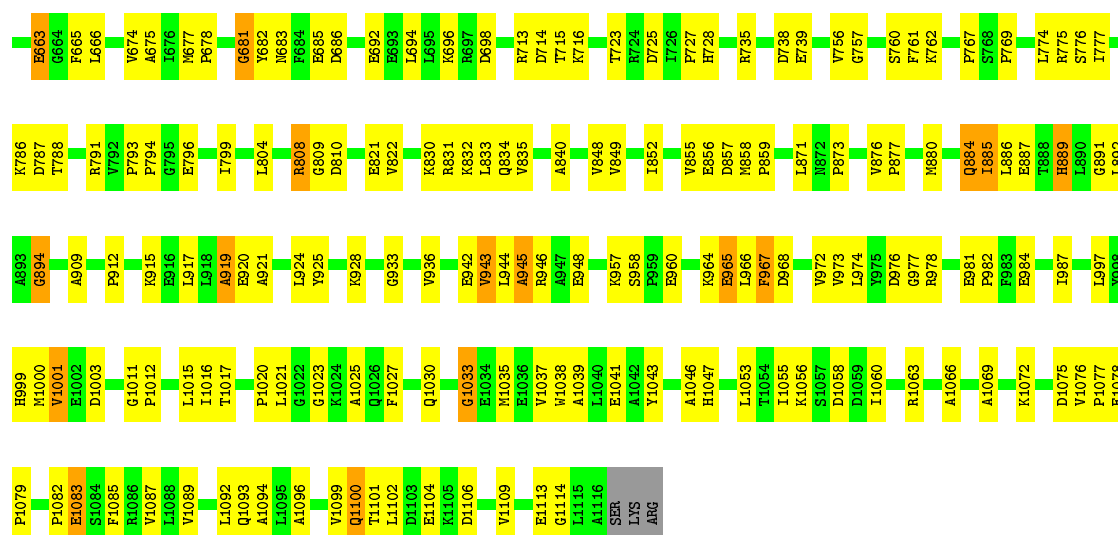


• Molecule 2: RNA POLYMERASE, BETA SUBUNIT

Chain C: 58% 34%

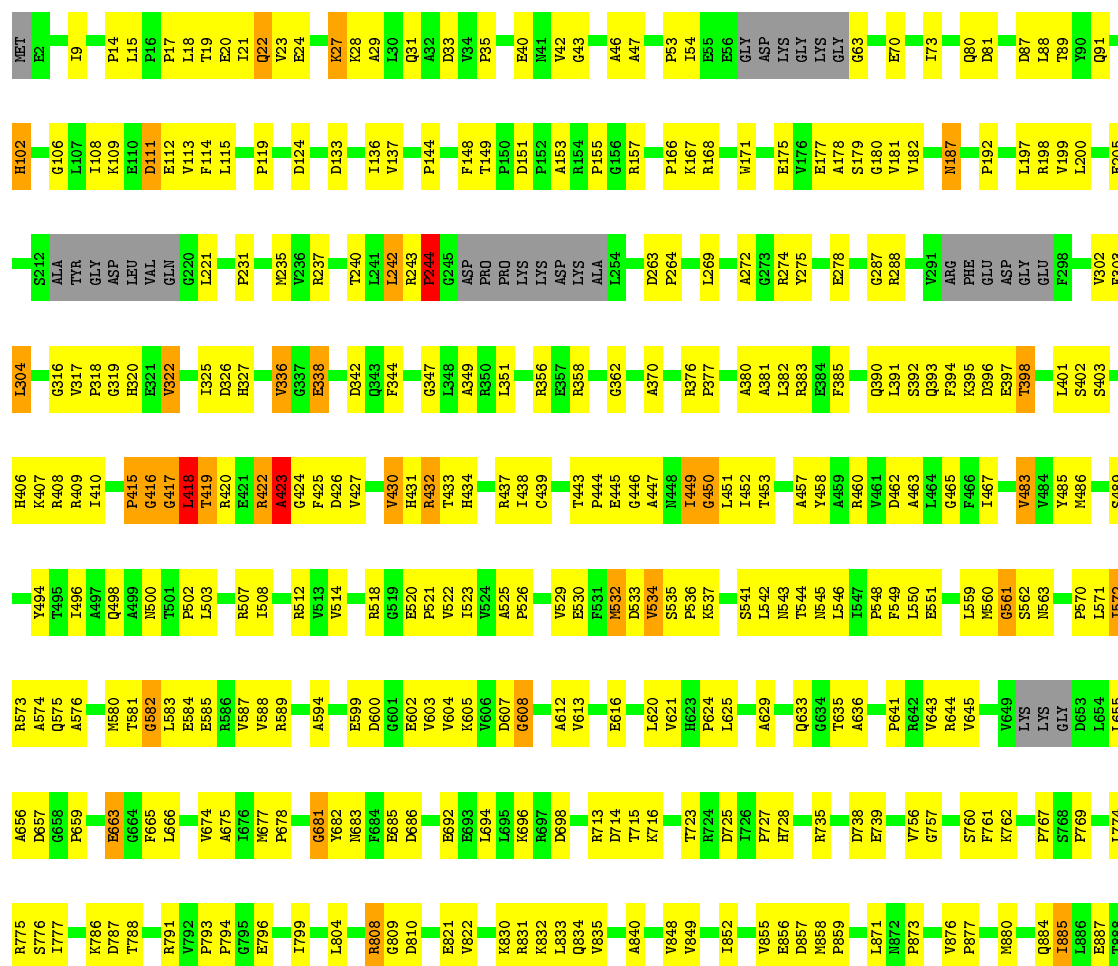


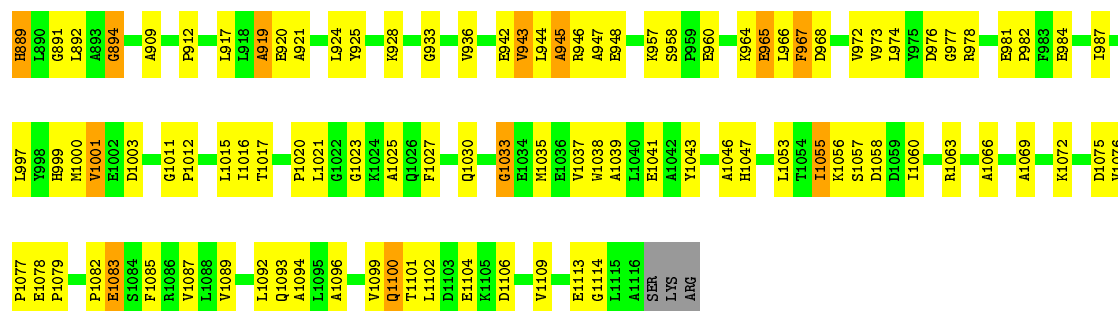




## • Molecule 2: RNA POLYMERASE, BETA SUBUNIT

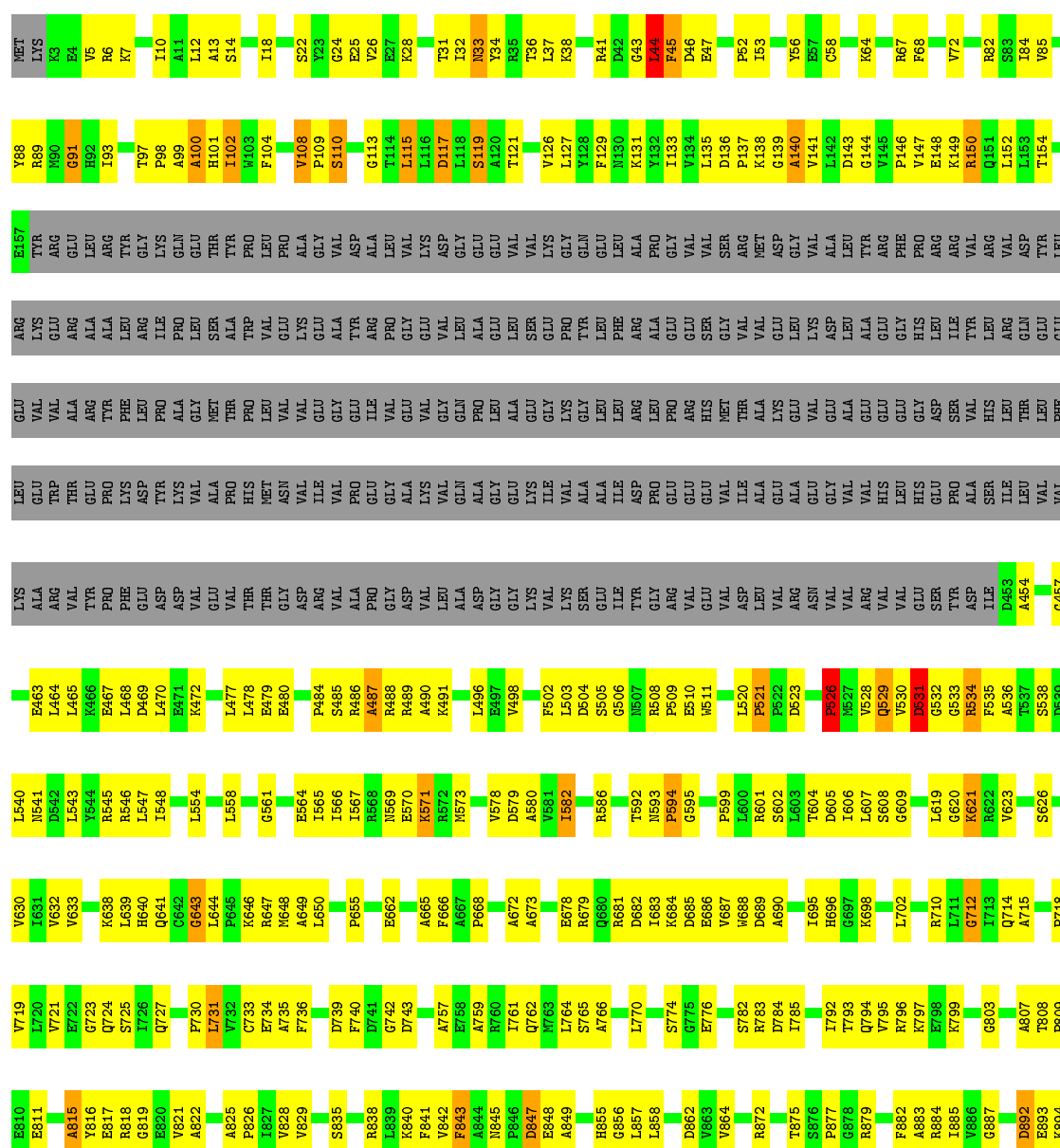
Chain L: 58% 35%

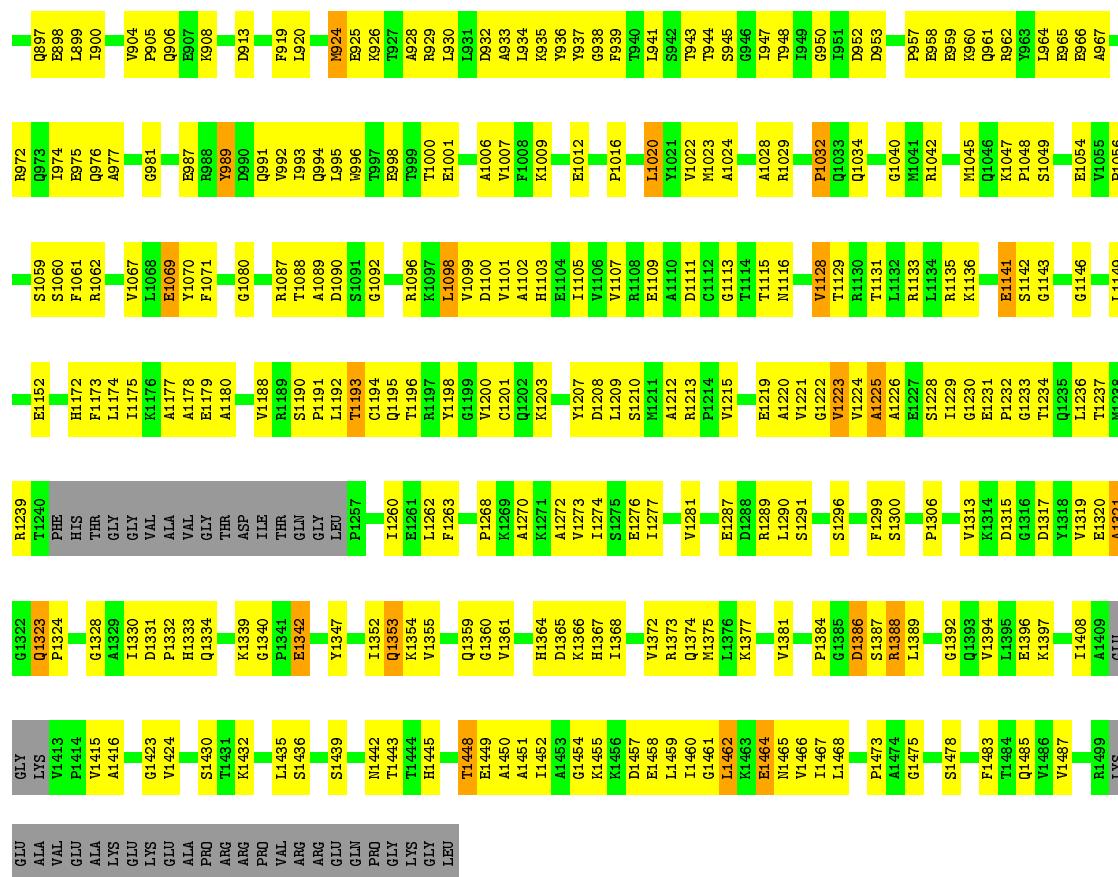




• Molecule 3: RNA POLYMERASE, BETA-PRIME SUBUNIT

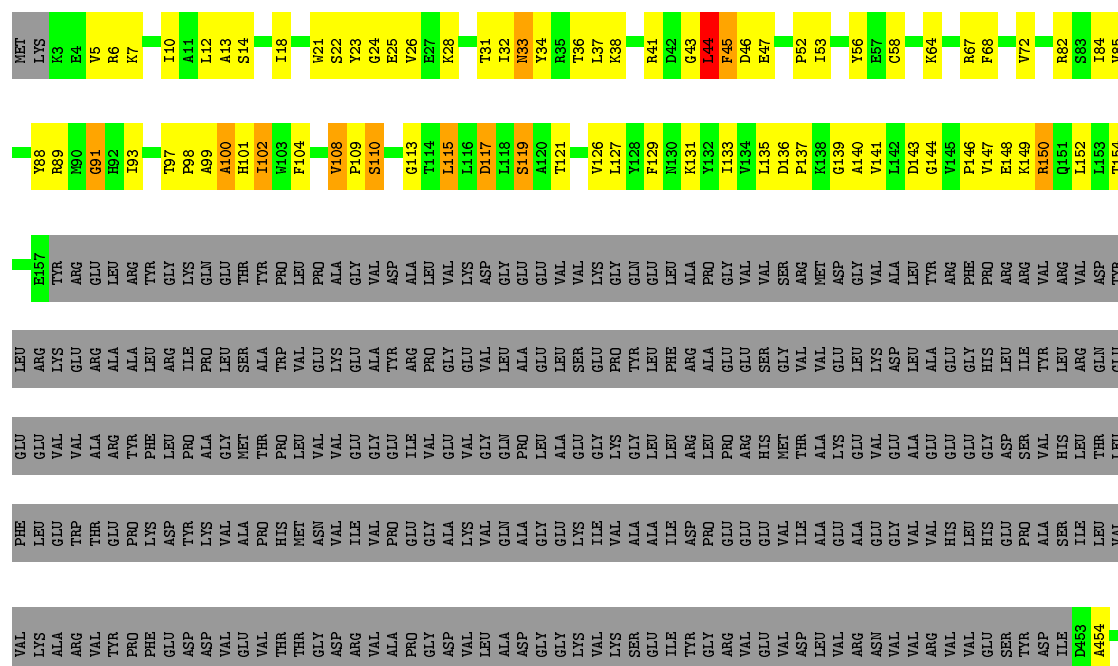
Chain D: 41% 33% 22%



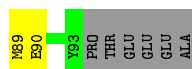


- Molecule 3: RNA POLYMERASE, BETA-PRIME SUBUNIT

Chain M:  41% 33% 1% 22%

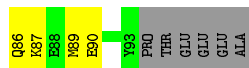






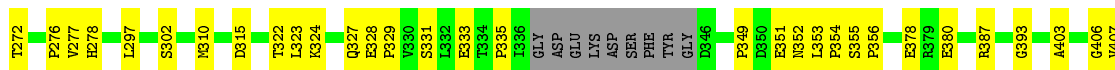
• Molecule 4: RNA POLYMERASE, OMEGA SUBUNIT

Chain N: 47% 44% 7%



• Molecule 5: SIGMA FACTOR SIGA

Chain H: 75% 21%



• Molecule 5: SIGMA FACTOR SIGA

Chain Q: 75% 21%



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	155.00Å 271.20Å 155.30Å 90.00° 91.40° 90.00°	Depositor
Resolution (Å)	(Not available) – 4.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-4.00)	Depositor
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program		Depositor
R, $R_{free}$	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	18756	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

## 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	0.37	0/671	1.02	0/670
1	B	0.36	0/659	1.11	0/658
1	J	0.37	0/671	1.02	0/670
1	K	0.36	0/659	1.11	0/658
2	C	0.85	9/3246 (0.3%)	1.37	15/3240 (0.5%)
2	L	0.85	9/3246 (0.3%)	1.37	15/3240 (0.5%)
3	D	0.94	21/3545 (0.6%)	1.34	21/3541 (0.6%)
3	M	0.94	21/3545 (0.6%)	1.34	21/3541 (0.6%)
4	E	0.34	0/275	0.87	0/274
4	N	0.34	0/275	0.87	0/274
5	H	0.59	3/964 (0.3%)	0.85	4/962 (0.4%)
5	Q	0.59	3/964 (0.3%)	0.85	4/962 (0.4%)
All	All	0.80	66/18720 (0.4%)	1.26	80/18690 (0.4%)

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
2	C	0	8
2	L	0	8
3	D	0	7
3	M	0	7
All	All	0	30

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	244	PRO	C-N	-22.34	0.92	1.33
2	L	244	PRO	C-N	-22.31	0.92	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	91	GLY	C-N	-18.07	0.92	1.34
3	M	91	GLY	C-N	-18.07	0.92	1.34
3	D	531	ASP	C-N	-17.95	1.00	1.33
3	M	531	ASP	C-N	-17.92	1.00	1.33
2	C	417	GLY	C-N	-16.64	0.95	1.34
2	L	417	GLY	C-N	-16.61	0.95	1.34
3	M	532	GLY	C-N	15.96	1.61	1.33
3	D	532	GLY	C-N	15.93	1.61	1.33
3	D	44	LEU	C-N	15.76	1.70	1.34
3	M	44	LEU	C-N	15.73	1.70	1.34
2	L	240	THR	C-N	-15.27	0.98	1.34
2	C	240	THR	C-N	-15.23	0.99	1.34
2	L	422	ARG	C-N	-14.27	1.01	1.34
2	C	419	THR	C-N	-14.27	1.01	1.34
2	L	418	LEU	C-N	-14.26	1.01	1.34
2	C	422	ARG	C-N	-14.24	1.01	1.34
2	L	419	THR	C-N	-14.24	1.01	1.34
2	C	418	LEU	C-N	-14.24	1.01	1.34
3	D	521	PRO	C-N	-13.31	1.08	1.34
3	M	521	PRO	C-N	-13.28	1.09	1.34
5	H	239	VAL	C-N	-12.30	1.05	1.34
5	Q	239	VAL	C-N	-12.27	1.05	1.34
3	D	529	GLN	C-N	-11.91	1.06	1.34
3	M	529	GLN	C-N	-11.90	1.06	1.34
2	L	423	ALA	C-N	-10.79	1.13	1.33
2	C	423	ALA	C-N	-10.75	1.13	1.33
3	M	526	PRO	C-N	-10.69	1.09	1.34
3	D	526	PRO	C-N	-10.66	1.09	1.34
3	D	533	GLY	C-N	10.19	1.57	1.34
3	M	533	GLY	C-N	10.19	1.57	1.34
3	D	1080	GLY	C-N	9.76	1.50	1.33
3	M	1080	GLY	C-N	9.74	1.50	1.33
3	D	1087	ARG	C-N	-9.68	1.11	1.34
3	M	1087	ARG	C-N	-9.65	1.11	1.34
3	D	113	GLY	C-N	-9.33	1.12	1.34
3	M	113	GLY	C-N	-9.30	1.12	1.34
3	D	115	LEU	C-N	-7.80	1.16	1.34
3	M	115	LEU	C-N	-7.79	1.16	1.34
3	M	113	GLY	N-CA	-7.71	1.34	1.46
3	D	113	GLY	N-CA	-7.70	1.34	1.46
3	D	538	SER	C-N	7.54	1.51	1.34
3	M	538	SER	C-N	7.53	1.51	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	416	GLY	C-N	-7.38	1.19	1.33
2	L	416	GLY	C-N	-7.34	1.19	1.33
3	M	528	VAL	C-N	7.15	1.50	1.34
3	D	528	VAL	C-N	7.14	1.50	1.34
3	D	93	ILE	C-N	-7.03	1.17	1.34
3	M	93	ILE	C-N	-7.03	1.17	1.34
5	H	238	ALA	N-CA	6.76	1.59	1.46
5	Q	238	ALA	N-CA	6.75	1.59	1.46
2	L	415	PRO	C-N	6.10	1.44	1.33
2	C	415	PRO	C-N	6.07	1.44	1.33
3	D	523	ASP	C-N	-5.78	1.20	1.34
3	M	523	ASP	C-N	-5.76	1.20	1.34
3	D	534	ARG	C-N	-5.72	1.20	1.34
3	M	534	ARG	C-N	-5.68	1.21	1.34
3	M	1089	ALA	C-N	-5.39	1.21	1.34
5	Q	234	GLY	CA-C	-5.39	1.43	1.51
3	D	1089	ALA	C-N	-5.39	1.21	1.34
5	H	234	GLY	CA-C	-5.36	1.43	1.51
3	M	88	TYR	C-N	5.30	1.46	1.34
3	D	88	TYR	C-N	5.29	1.46	1.34
3	D	1096	ARG	C-N	-5.11	1.22	1.34
3	M	1096	ARG	C-N	-5.09	1.22	1.34

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	244	PRO	CA-C-N	24.93	166.06	116.20
2	C	244	PRO	CA-C-N	24.90	166.00	116.20
2	L	417	GLY	C-N-CA	20.66	173.35	121.70
2	C	417	GLY	C-N-CA	20.66	173.34	121.70
3	D	531	ASP	CA-C-N	19.67	155.53	116.20
3	M	531	ASP	CA-C-N	19.63	155.46	116.20
2	C	419	THR	C-N-CA	19.39	170.16	121.70
2	L	419	THR	C-N-CA	19.38	170.14	121.70
3	M	534	ARG	C-N-CA	18.67	168.37	121.70
3	D	534	ARG	C-N-CA	18.66	168.35	121.70
2	C	244	PRO	C-N-CA	17.86	159.81	122.30
2	L	244	PRO	C-N-CA	17.85	159.78	122.30
3	D	529	GLN	C-N-CA	15.36	160.09	121.70
3	M	529	GLN	C-N-CA	15.34	160.05	121.70
2	C	242	LEU	C-N-CA	14.61	158.21	121.70
2	L	242	LEU	C-N-CA	14.61	158.22	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	422	ARG	C-N-CA	14.25	157.32	121.70
2	L	422	ARG	C-N-CA	14.25	157.32	121.70
2	C	422	ARG	CA-C-N	14.14	148.30	117.20
2	L	422	ARG	CA-C-N	14.11	148.25	117.20
3	D	531	ASP	C-N-CA	13.62	150.90	122.30
3	M	531	ASP	C-N-CA	13.62	150.90	122.30
2	L	417	GLY	CA-C-N	13.47	146.84	117.20
2	C	417	GLY	CA-C-N	13.47	146.84	117.20
3	D	91	GLY	CA-C-N	13.04	145.89	117.20
3	M	91	GLY	CA-C-N	13.04	145.89	117.20
3	M	526	PRO	C-N-CA	11.58	150.64	121.70
3	D	526	PRO	C-N-CA	11.57	150.64	121.70
2	L	418	LEU	C-N-CA	10.82	148.75	121.70
2	C	418	LEU	C-N-CA	10.80	148.71	121.70
3	D	534	ARG	CA-C-N	10.79	140.93	117.20
3	M	534	ARG	CA-C-N	10.78	140.91	117.20
3	D	91	GLY	C-N-CA	10.65	148.32	121.70
3	M	91	GLY	C-N-CA	10.65	148.32	121.70
3	D	88	TYR	C-N-CA	-10.27	96.02	121.70
3	M	88	TYR	C-N-CA	-10.26	96.06	121.70
3	D	526	PRO	CA-C-N	10.03	139.26	117.20
3	M	526	PRO	CA-C-N	10.03	139.26	117.20
3	D	88	TYR	CA-C-N	-9.85	95.53	117.20
3	M	88	TYR	CA-C-N	-9.85	95.54	117.20
3	M	532	GLY	CA-C-N	9.51	135.22	116.20
3	D	532	GLY	CA-C-N	9.50	135.20	116.20
2	L	418	LEU	CA-C-N	8.52	135.95	117.20
2	C	418	LEU	CA-C-N	8.49	135.89	117.20
2	C	242	LEU	CA-C-N	7.84	134.45	117.20
2	L	242	LEU	CA-C-N	7.84	134.45	117.20
3	D	1088	THR	C-N-CA	7.80	141.20	121.70
3	M	1088	THR	C-N-CA	7.79	141.17	121.70
5	H	225	LEU	CA-C-N	6.65	131.84	117.20
5	Q	225	LEU	CA-C-N	6.65	131.83	117.20
2	L	423	ALA	CA-C-N	6.59	129.39	116.20
2	C	423	ALA	CA-C-N	6.59	129.38	116.20
3	M	1128	VAL	N-CA-C	-6.48	93.50	111.00
3	D	1128	VAL	N-CA-C	-6.47	93.52	111.00
3	D	113	GLY	CA-C-N	6.34	131.14	117.20
3	M	113	GLY	CA-C-N	6.32	131.11	117.20
5	H	173	GLU	N-CA-C	6.20	127.74	111.00
5	Q	173	GLU	N-CA-C	6.19	127.72	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1080	GLY	CA-C-N	-6.11	103.98	116.20
3	M	1080	GLY	CA-C-N	-6.11	103.98	116.20
2	C	416	GLY	CA-C-N	6.09	128.38	116.20
2	L	416	GLY	CA-C-N	6.07	128.34	116.20
3	D	93	ILE	C-N-CA	6.06	136.85	121.70
3	M	93	ILE	C-N-CA	6.05	136.83	121.70
3	D	44	LEU	C-N-CA	-6.01	106.66	121.70
2	C	416	GLY	C-N-CA	6.01	134.92	122.30
3	M	44	LEU	C-N-CA	-6.01	106.68	121.70
2	L	416	GLY	C-N-CA	6.00	134.89	122.30
2	C	419	THR	CA-C-N	5.63	129.58	117.20
2	L	419	THR	CA-C-N	5.62	129.57	117.20
3	D	536	ALA	N-CA-C	5.50	125.84	111.00
3	M	536	ALA	N-CA-C	5.49	125.83	111.00
5	H	225	LEU	C-N-CA	5.46	135.36	121.70
5	Q	225	LEU	C-N-CA	5.46	135.36	121.70
3	M	89	ARG	C-N-CA	-5.24	108.61	121.70
5	Q	239	VAL	CA-C-N	-5.24	105.68	117.20
3	D	89	ARG	C-N-CA	-5.23	108.63	121.70
5	H	239	VAL	CA-C-N	-5.23	105.70	117.20
3	D	521	PRO	CA-C-N	5.14	131.49	117.10
3	M	521	PRO	CA-C-N	5.13	131.48	117.10

There are no chirality outliers.

All (30) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	242	LEU	Peptide
2	C	244	PRO	Peptide
2	C	416	GLY	Peptide
2	C	417	GLY	Peptide
2	C	418	LEU	Peptide
2	C	419	THR	Peptide
2	C	422	ARG	Peptide
2	C	423	ALA	Peptide
3	D	115	LEU	Peptide
3	D	521	PRO	Peptide
3	D	526	PRO	Peptide
3	D	529	GLN	Peptide
3	D	531	ASP	Peptide
3	D	534	ARG	Peptide
3	D	91	GLY	Peptide

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Mol	Chain	Res	Type	Group
2	L	242	LEU	Peptide
2	L	244	PRO	Peptide
2	L	416	GLY	Peptide
2	L	417	GLY	Peptide
2	L	418	LEU	Peptide
2	L	419	THR	Peptide
2	L	422	ARG	Peptide
2	L	423	ALA	Peptide
3	M	115	LEU	Peptide
3	M	521	PRO	Peptide
3	M	526	PRO	Peptide
3	M	529	GLN	Peptide
3	M	531	ASP	Peptide
3	M	534	ARG	Peptide
3	M	91	GLY	Peptide

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	672	0	241	13	0
1	B	660	0	238	10	0
1	J	672	0	241	13	0
1	K	660	0	238	9	0
2	C	3252	0	1190	105	0
2	L	3252	0	1190	107	0
3	D	3549	0	1280	135	0
3	M	3549	0	1280	134	0
4	E	276	0	96	14	0
4	N	276	0	96	15	0
5	H	966	0	342	14	0
5	Q	966	0	342	14	0
6	D	1	0	0	0	0
6	M	1	0	0	0	0
7	D	2	0	0	0	0
7	M	2	0	0	0	0
All	All	18756	0	6774	571	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 22.

All (571) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:44:LEU:C	3:D:45:PHE:N	1.70	1.42
3:M:44:LEU:C	3:M:45:PHE:N	1.70	1.41
3:M:933:ALA:C	3:M:935:LYS:H	1.80	0.83
2:L:1033:GLY:HA2	3:M:620:GLY:HA2	1.60	0.82
2:L:542:LEU:C	2:L:544:THR:H	1.83	0.82
2:C:1033:GLY:HA2	3:D:620:GLY:HA2	1.60	0.82
3:D:933:ALA:C	3:D:935:LYS:H	1.81	0.81
2:C:1033:GLY:CA	3:D:620:GLY:HA2	2.10	0.81
2:L:1033:GLY:CA	3:M:620:GLY:HA2	2.10	0.81
2:C:542:LEU:C	2:C:544:THR:H	1.83	0.80
3:D:152:LEU:C	3:D:154:THR:H	1.85	0.80
3:D:44:LEU:C	3:D:46:ASP:H	1.85	0.80
3:M:44:LEU:C	3:M:46:ASP:H	1.85	0.79
2:L:533:ASP:C	2:L:535:SER:H	1.86	0.78
2:C:533:ASP:C	2:C:535:SER:H	1.86	0.78
3:D:578:VAL:C	3:D:580:ALA:H	1.87	0.78
2:C:681:GLY:C	2:C:683:ASN:H	1.88	0.77
3:M:578:VAL:C	3:M:580:ALA:H	1.87	0.77
3:M:152:LEU:C	3:M:154:THR:H	1.85	0.77
3:D:1069:GLU:C	3:D:1071:PHE:H	1.89	0.76
2:C:349:ALA:C	2:C:351:LEU:H	1.89	0.76
2:L:559:LEU:C	2:L:561:GLY:H	1.89	0.76
3:D:44:LEU:C	3:D:45:PHE:CA	2.54	0.76
2:C:559:LEU:C	2:C:561:GLY:H	1.89	0.76
3:M:1069:GLU:C	3:M:1071:PHE:H	1.89	0.76
3:M:44:LEU:C	3:M:45:PHE:CA	2.53	0.76
2:L:349:ALA:C	2:L:351:LEU:H	1.89	0.75
2:L:681:GLY:C	2:L:683:ASN:H	1.88	0.75
5:H:151:LEU:C	5:H:153:THR:H	1.93	0.72
2:L:383:ARG:C	2:L:385:PHE:H	1.93	0.71
3:M:604:THR:C	3:M:606:ILE:H	1.94	0.71
2:C:383:ARG:C	2:C:385:PHE:H	1.93	0.71
3:D:604:THR:C	3:D:606:ILE:H	1.94	0.70
5:Q:151:LEU:C	5:Q:153:THR:H	1.93	0.70
3:D:1022:VAL:C	3:D:1024:ALA:H	1.96	0.69
2:L:1100:GLN:C	2:L:1102:LEU:H	1.97	0.69
3:M:975:GLU:C	3:M:977:ALA:H	1.96	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:544:THR:C	2:L:546:LEU:H	1.97	0.68
2:C:1100:GLN:C	2:C:1102:LEU:H	1.97	0.68
3:D:975:GLU:C	3:D:977:ALA:H	1.96	0.67
3:M:1022:VAL:C	3:M:1024:ALA:H	1.96	0.67
2:C:1092:LEU:C	2:C:1094:ALA:H	1.97	0.67
2:C:544:THR:C	2:C:546:LEU:H	1.97	0.67
5:H:276:PRO:C	5:H:278:HIS:H	1.98	0.67
2:C:1092:LEU:C	2:C:1094:ALA:N	2.48	0.67
2:L:1092:LEU:C	2:L:1094:ALA:N	2.48	0.67
4:E:25:LYS:C	4:E:27:ALA:H	1.98	0.67
3:D:1060:SER:C	3:D:1062:ARG:H	1.98	0.66
2:C:347:GLY:C	2:C:349:ALA:H	1.99	0.66
4:N:25:LYS:C	4:N:27:ALA:H	1.98	0.66
3:M:1060:SER:C	3:M:1062:ARG:H	1.98	0.65
2:L:1092:LEU:C	2:L:1094:ALA:H	1.97	0.65
2:L:347:GLY:C	2:L:349:ALA:H	1.99	0.65
2:L:406:HIS:C	2:L:408:ARG:H	2.01	0.65
3:M:1448:THR:C	3:M:1450:ALA:H	2.01	0.65
3:M:933:ALA:C	3:M:935:LYS:N	2.50	0.64
5:Q:276:PRO:C	5:Q:278:HIS:H	1.98	0.64
3:D:1448:THR:C	3:D:1450:ALA:H	2.01	0.64
3:D:734:GLU:C	3:D:736:PHE:H	2.01	0.64
2:C:542:LEU:C	2:C:544:THR:N	2.51	0.63
2:L:542:LEU:C	2:L:544:THR:N	2.51	0.63
2:L:437:ARG:C	2:L:439:CYS:H	2.02	0.63
3:M:734:GLU:C	3:M:736:PHE:H	2.01	0.63
2:C:406:HIS:C	2:C:408:ARG:H	2.01	0.63
3:M:1191:PRO:C	3:M:1193:THR:H	2.01	0.63
2:C:430:VAL:C	2:C:432:ARG:H	2.02	0.63
2:C:437:ARG:C	2:C:439:CYS:H	2.02	0.63
2:L:430:VAL:C	2:L:432:ARG:H	2.02	0.62
3:D:1191:PRO:C	3:D:1193:THR:H	2.01	0.62
2:L:1100:GLN:C	2:L:1102:LEU:N	2.53	0.62
3:M:957:PRO:C	3:M:959:GLU:H	2.03	0.62
4:E:70:THR:C	4:E:72:ARG:H	2.02	0.62
5:H:270:ALA:C	5:H:272:THR:H	2.02	0.62
3:D:44:LEU:CA	3:D:45:PHE:N	2.62	0.62
3:D:957:PRO:C	3:D:959:GLU:H	2.03	0.62
2:L:523:ILE:C	2:L:525:ALA:N	2.51	0.61
2:L:549:PHE:C	2:L:551:GLU:H	2.03	0.61
3:M:643:GLY:HA3	3:M:727:GLN:H	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:70:THR:C	4:N:72:ARG:H	2.02	0.61
3:D:643:GLY:HA3	3:D:727:GLN:H	1.65	0.61
3:M:44:LEU:CA	3:M:45:PHE:N	2.62	0.61
2:C:561:GLY:C	2:C:563:ASN:H	2.04	0.61
5:Q:270:ALA:C	5:Q:272:THR:H	2.02	0.61
3:M:855:HIS:C	3:M:857:LEU:H	2.04	0.61
3:D:855:HIS:C	3:D:857:LEU:H	2.04	0.61
2:L:450:GLY:C	2:L:452:ILE:H	2.04	0.61
3:M:152:LEU:C	3:M:154:THR:N	2.54	0.61
2:L:561:GLY:C	2:L:563:ASN:H	2.04	0.61
2:C:1100:GLN:C	2:C:1102:LEU:N	2.53	0.60
4:E:11:GLY:C	4:E:13:VAL:H	2.05	0.60
3:M:757:ALA:C	3:M:759:ALA:H	2.04	0.60
4:N:11:GLY:C	4:N:13:VAL:H	2.05	0.60
2:C:549:PHE:C	2:C:551:GLU:H	2.03	0.60
2:L:681:GLY:C	2:L:683:ASN:N	2.55	0.60
3:M:688:TRP:C	3:M:690:ALA:H	2.05	0.60
2:C:450:GLY:C	2:C:452:ILE:H	2.04	0.60
2:C:178:ALA:C	2:C:180:GLY:H	2.05	0.59
3:M:639:LEU:C	3:M:641:GLN:H	2.05	0.59
3:D:688:TRP:C	3:D:690:ALA:H	2.05	0.59
3:M:119:SER:C	3:M:121:THR:H	2.05	0.59
2:C:559:LEU:C	2:C:561:GLY:N	2.55	0.59
2:L:178:ALA:C	2:L:180:GLY:H	2.05	0.59
2:C:406:HIS:C	2:C:408:ARG:N	2.55	0.59
3:D:757:ALA:C	3:D:759:ALA:H	2.04	0.59
3:M:503:LEU:C	3:M:505:SER:H	2.06	0.59
3:M:845:ASN:C	3:M:847:ASP:H	2.06	0.59
3:M:1141:GLU:C	3:M:1143:GLY:H	2.06	0.59
3:D:639:LEU:C	3:D:641:GLN:H	2.05	0.59
2:L:325:ILE:C	2:L:327:HIS:H	2.06	0.59
3:D:44:LEU:C	3:D:46:ASP:N	2.56	0.59
2:L:559:LEU:C	2:L:561:GLY:N	2.55	0.59
3:M:1340:GLY:C	3:M:1342:GLU:H	2.06	0.59
3:M:578:VAL:C	3:M:580:ALA:N	2.56	0.59
2:C:581:THR:C	2:C:583:LEU:H	2.06	0.59
3:D:119:SER:C	3:D:121:THR:H	2.05	0.59
3:D:1226:ALA:C	3:D:1228:SER:H	2.06	0.59
2:L:581:THR:C	2:L:583:LEU:H	2.06	0.59
2:C:483:VAL:C	2:C:485:TYR:H	2.07	0.58
3:D:1340:GLY:C	3:D:1342:GLU:H	2.07	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:503:LEU:C	3:D:505:SER:H	2.06	0.58
2:L:349:ALA:C	2:L:351:LEU:N	2.56	0.58
2:C:111:ASP:C	2:C:113:VAL:H	2.07	0.58
2:C:808:ARG:C	2:C:810:ASP:H	2.07	0.58
2:L:406:HIS:C	2:L:408:ARG:N	2.55	0.58
2:C:325:ILE:C	2:C:327:HIS:H	2.06	0.58
2:C:424:GLY:C	2:C:426:ASP:H	2.06	0.58
1:A:217:ILE:C	1:A:219:LYS:H	2.06	0.58
2:L:424:GLY:C	2:L:426:ASP:H	2.06	0.58
2:C:523:ILE:C	2:C:525:ALA:N	2.51	0.58
3:D:1032:PRO:C	3:D:1034:GLN:H	2.08	0.58
2:L:808:ARG:C	2:L:810:ASP:H	2.07	0.58
2:L:885:ILE:C	2:L:887:GLU:N	2.56	0.58
3:M:1032:PRO:C	3:M:1034:GLN:H	2.07	0.58
3:D:119:SER:C	3:D:121:THR:N	2.58	0.58
3:D:933:ALA:C	3:D:935:LYS:N	2.50	0.58
3:M:44:LEU:C	3:M:46:ASP:N	2.55	0.58
3:D:467:GLU:C	3:D:469:ASP:H	2.08	0.57
3:D:578:VAL:C	3:D:580:ALA:N	2.56	0.57
2:L:533:ASP:C	2:L:535:SER:N	2.57	0.57
3:M:108:VAL:C	3:M:110:SER:N	2.57	0.57
3:D:845:ASN:C	3:D:847:ASP:N	2.58	0.57
2:L:111:ASP:C	2:L:113:VAL:H	2.07	0.57
3:D:845:ASN:C	3:D:847:ASP:H	2.05	0.57
3:D:877:PRO:C	3:D:879:ARG:H	2.08	0.57
2:L:1015:LEU:C	2:L:1017:THR:H	2.08	0.57
3:M:1226:ALA:C	3:M:1228:SER:H	2.06	0.57
3:M:509:PRO:C	3:M:511:TRP:H	2.08	0.57
2:C:533:ASP:C	2:C:535:SER:N	2.57	0.57
2:C:885:ILE:C	2:C:887:GLU:N	2.56	0.57
2:C:943:VAL:C	2:C:945:ALA:N	2.58	0.57
1:J:217:ILE:C	1:J:219:LYS:H	2.06	0.57
3:M:467:GLU:C	3:M:469:ASP:H	2.08	0.57
3:M:845:ASN:C	3:M:847:ASP:N	2.58	0.57
2:C:349:ALA:C	2:C:351:LEU:N	2.56	0.56
2:L:1033:GLY:HA3	3:M:620:GLY:HA2	1.86	0.56
3:M:117:ASP:C	3:M:119:SER:H	2.07	0.56
3:D:1069:GLU:C	3:D:1071:PHE:N	2.58	0.56
3:D:1141:GLU:C	3:D:1143:GLY:H	2.06	0.56
3:M:924:MET:C	3:M:926:LYS:H	2.09	0.56
2:C:1015:LEU:C	2:C:1017:THR:H	2.08	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:117:ASP:C	3:D:119:SER:H	2.07	0.56
3:D:924:MET:C	3:D:926:LYS:H	2.09	0.56
3:M:119:SER:C	3:M:121:THR:N	2.58	0.56
2:C:383:ARG:C	2:C:385:PHE:N	2.59	0.56
2:C:681:GLY:C	2:C:683:ASN:N	2.55	0.56
2:L:383:ARG:C	2:L:385:PHE:N	2.59	0.56
2:C:1023:GLY:C	2:C:1025:ALA:H	2.09	0.56
2:L:483:VAL:C	2:L:485:TYR:H	2.07	0.56
2:L:889:HIS:C	2:L:891:GLY:N	2.58	0.56
2:L:943:VAL:C	2:L:945:ALA:N	2.58	0.56
3:M:1069:GLU:C	3:M:1071:PHE:N	2.58	0.56
2:C:889:HIS:C	2:C:891:GLY:N	2.58	0.56
5:H:151:LEU:C	5:H:153:THR:N	2.59	0.56
2:C:424:GLY:C	2:C:426:ASP:N	2.58	0.56
2:C:1033:GLY:HA3	3:D:620:GLY:HA2	1.86	0.56
2:L:424:GLY:C	2:L:426:ASP:N	2.58	0.56
2:C:885:ILE:C	2:C:887:GLU:H	2.09	0.55
3:D:108:VAL:C	3:D:110:SER:N	2.58	0.55
3:M:487:ALA:C	3:M:489:ARG:H	2.10	0.55
3:M:877:PRO:C	3:M:879:ARG:H	2.08	0.55
1:A:71:VAL:H	2:C:608:GLY:CA	2.20	0.55
3:D:509:PRO:C	3:D:511:TRP:H	2.08	0.55
2:L:1023:GLY:C	2:L:1025:ALA:H	2.09	0.55
2:C:380:ALA:C	2:C:382:LEU:H	2.10	0.55
2:C:570:PRO:C	2:C:572:ILE:H	2.09	0.55
2:L:447:ALA:C	2:L:449:ILE:H	2.10	0.55
1:J:71:VAL:H	2:L:608:GLY:CA	2.20	0.55
3:M:1289:ARG:C	3:M:1291:SER:H	2.10	0.54
2:L:885:ILE:C	2:L:887:GLU:H	2.09	0.54
3:D:1332:PRO:C	3:D:1334:GLN:H	2.10	0.54
2:L:380:ALA:C	2:L:382:LEU:H	2.10	0.54
3:D:993:ILE:C	3:D:995:LEU:H	2.11	0.54
3:M:1022:VAL:C	3:M:1024:ALA:N	2.61	0.54
3:D:1289:ARG:C	3:D:1291:SER:H	2.10	0.54
2:L:570:PRO:C	2:L:572:ILE:H	2.09	0.54
2:L:356:ARG:C	2:L:358:ARG:H	2.11	0.54
3:D:1022:VAL:C	3:D:1024:ALA:N	2.61	0.54
1:J:217:ILE:C	1:J:219:LYS:N	2.61	0.54
1:A:217:ILE:C	1:A:219:LYS:N	2.61	0.54
3:D:152:LEU:C	3:D:154:THR:N	2.54	0.54
3:D:487:ALA:C	3:D:489:ARG:H	2.10	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:VAL:C	1:B:36:LEU:N	2.61	0.53
2:L:892:LEU:C	2:L:894:GLY:H	2.12	0.53
2:C:571:LEU:C	2:C:573:ARG:H	2.11	0.53
2:L:336:VAL:C	2:L:338:GLU:H	2.11	0.53
2:L:532:MET:C	2:L:534:VAL:H	2.12	0.53
2:C:447:ALA:C	2:C:449:ILE:H	2.10	0.53
2:C:892:LEU:C	2:C:894:GLY:H	2.12	0.53
1:K:34:VAL:C	1:K:36:LEU:N	2.61	0.53
3:M:1340:GLY:C	3:M:1342:GLU:N	2.62	0.53
2:L:571:LEU:C	2:L:573:ARG:H	2.11	0.53
3:M:993:ILE:C	3:M:995:LEU:H	2.11	0.53
3:D:465:LEU:C	3:D:467:GLU:H	2.12	0.52
3:M:470:LEU:C	3:M:472:LYS:H	2.13	0.52
2:C:336:VAL:C	2:C:338:GLU:H	2.11	0.52
1:K:105:GLY:HA2	1:K:136:GLY:HA3	1.91	0.52
3:M:1332:PRO:C	3:M:1334:GLN:H	2.11	0.52
2:L:544:THR:C	2:L:546:LEU:N	2.63	0.52
2:C:356:ARG:C	2:C:358:ARG:H	2.11	0.52
3:D:685:ASP:C	3:D:687:VAL:H	2.13	0.52
2:C:532:MET:C	2:C:534:VAL:H	2.12	0.52
3:M:604:THR:C	3:M:606:ILE:N	2.62	0.52
1:J:79:ILE:C	1:J:81:ASN:H	2.13	0.52
3:M:685:ASP:C	3:M:687:VAL:H	2.13	0.52
5:Q:151:LEU:C	5:Q:153:THR:N	2.59	0.52
1:A:79:ILE:C	1:A:81:ASN:H	2.13	0.52
3:D:924:MET:C	3:D:926:LYS:N	2.64	0.52
1:B:105:GLY:HA2	1:B:136:GLY:HA3	1.91	0.51
3:D:1196:THR:C	3:D:1198:TYR:H	2.12	0.51
3:D:541:ASN:C	3:D:543:LEU:N	2.61	0.51
5:Q:322:THR:C	5:Q:324:LYS:H	2.14	0.51
3:D:1020:LEU:C	3:D:1022:VAL:H	2.14	0.51
3:D:1340:GLY:C	3:D:1342:GLU:N	2.62	0.51
3:D:604:THR:C	3:D:606:ILE:N	2.62	0.51
3:M:924:MET:C	3:M:926:LYS:N	2.64	0.51
3:M:465:LEU:C	3:M:467:GLU:H	2.12	0.51
3:M:102:ILE:C	3:M:104:PHE:N	2.64	0.51
5:H:322:THR:C	5:H:324:LYS:H	2.14	0.51
3:M:1196:THR:C	3:M:1198:TYR:H	2.12	0.51
2:C:544:THR:C	2:C:546:LEU:N	2.63	0.51
3:M:1332:PRO:C	3:M:1334:GLN:N	2.64	0.51
3:D:108:VAL:C	3:D:110:SER:H	2.14	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:919:ALA:C	2:L:921:ALA:N	2.64	0.51
3:M:1020:LEU:C	3:M:1022:VAL:H	2.14	0.51
3:D:960:LYS:C	3:D:962:ARG:H	2.15	0.50
2:L:1041:GLU:C	2:L:1043:TYR:N	2.64	0.50
2:C:396:ASP:C	2:C:398:THR:H	2.15	0.50
2:C:723:THR:C	2:C:725:ASP:H	2.14	0.50
3:M:950:GLY:C	3:M:952:ASP:N	2.63	0.50
3:M:957:PRO:C	3:M:959:GLU:N	2.65	0.50
3:M:960:LYS:C	3:M:962:ARG:H	2.15	0.50
3:D:1332:PRO:C	3:D:1334:GLN:N	2.64	0.50
3:D:960:LYS:C	3:D:962:ARG:N	2.65	0.50
1:J:223:ASN:C	1:J:225:PHE:N	2.65	0.50
2:L:723:THR:C	2:L:725:ASP:H	2.15	0.50
2:C:581:THR:C	2:C:583:LEU:N	2.65	0.50
3:D:470:LEU:C	3:D:472:LYS:H	2.13	0.50
3:D:957:PRO:C	3:D:959:GLU:N	2.65	0.50
2:L:302:VAL:C	2:L:304:LEU:H	2.15	0.50
3:M:108:VAL:C	3:M:110:SER:H	2.14	0.50
3:M:960:LYS:C	3:M:962:ARG:N	2.65	0.50
2:L:396:ASP:C	2:L:398:THR:H	2.15	0.50
2:C:111:ASP:C	2:C:113:VAL:N	2.65	0.50
2:C:198:ARG:C	2:C:200:LEU:H	2.15	0.50
3:D:1331:ASP:C	3:D:1333:HIS:N	2.65	0.50
2:L:523:ILE:C	2:L:525:ALA:H	2.15	0.50
3:M:541:ASN:C	3:M:543:LEU:N	2.61	0.50
2:C:523:ILE:C	2:C:525:ALA:H	2.15	0.49
3:D:950:GLY:C	3:D:952:ASP:N	2.63	0.49
1:J:70:GLY:HA3	1:J:135:GLY:HA3	1.93	0.49
5:Q:276:PRO:C	5:Q:278:HIS:N	2.65	0.49
1:A:223:ASN:C	1:A:225:PHE:N	2.65	0.49
2:C:302:VAL:C	2:C:304:LEU:H	2.15	0.49
2:L:892:LEU:C	2:L:894:GLY:N	2.66	0.49
3:D:1223:VAL:C	3:D:1225:ALA:N	2.65	0.49
1:B:31:GLY:C	1:B:33:GLY:H	2.15	0.49
2:L:111:ASP:C	2:L:113:VAL:N	2.65	0.49
1:A:70:GLY:HA3	1:A:135:GLY:HA3	1.93	0.49
2:C:1041:GLU:C	2:C:1043:TYR:N	2.64	0.49
2:L:581:THR:C	2:L:583:LEU:N	2.65	0.49
3:M:975:GLU:C	3:M:977:ALA:N	2.65	0.49
2:C:919:ALA:C	2:C:921:ALA:N	2.64	0.49
2:L:774:LEU:C	2:L:776:SER:N	2.66	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:593:ASN:CA	3:M:594:PRO:C	2.81	0.49
2:L:198:ARG:C	2:L:200:LEU:H	2.15	0.49
3:M:1331:ASP:C	3:M:1333:HIS:N	2.65	0.49
2:C:89:THR:C	2:C:91:GLN:H	2.17	0.49
3:D:34:TYR:C	3:D:36:THR:N	2.66	0.49
2:C:774:LEU:C	2:C:776:SER:N	2.66	0.48
4:N:25:LYS:C	4:N:27:ALA:N	2.66	0.48
2:C:892:LEU:C	2:C:894:GLY:N	2.66	0.48
3:D:593:ASN:CA	3:D:594:PRO:C	2.81	0.48
3:M:989:TYR:C	3:M:991:GLN:N	2.66	0.48
3:D:1228:SER:C	3:D:1230:GLY:H	2.16	0.48
2:C:532:MET:C	2:C:534:VAL:N	2.67	0.48
1:K:31:GLY:C	1:K:33:GLY:H	2.15	0.48
2:L:532:MET:C	2:L:534:VAL:N	2.67	0.48
1:B:172:SER:C	1:B:174:VAL:H	2.17	0.48
3:D:975:GLU:C	3:D:977:ALA:N	2.65	0.48
2:L:1033:GLY:HA2	3:M:620:GLY:CA	2.37	0.48
2:L:89:THR:C	2:L:91:GLN:H	2.16	0.48
3:M:1228:SER:C	3:M:1230:GLY:H	2.16	0.48
2:C:27:LYS:C	2:C:29:ALA:N	2.67	0.48
3:M:34:TYR:C	3:M:36:THR:N	2.66	0.48
1:K:223:ASN:C	1:K:225:PHE:H	2.17	0.48
2:C:1085:PHE:C	2:C:1087:VAL:N	2.66	0.48
3:M:1223:VAL:C	3:M:1225:ALA:N	2.65	0.48
2:L:1085:PHE:C	2:L:1087:VAL:N	2.66	0.48
3:M:100:ALA:C	3:M:102:ILE:H	2.18	0.47
3:M:1226:ALA:C	3:M:1228:SER:N	2.68	0.47
3:M:710:ARG:C	3:M:712:GLY:N	2.65	0.47
1:A:122:ILE:C	1:A:124:ASN:H	2.18	0.47
3:D:1141:GLU:C	3:D:1143:GLY:N	2.68	0.47
4:E:25:LYS:C	4:E:27:ALA:N	2.66	0.47
1:B:223:ASN:C	1:B:225:PHE:H	2.17	0.47
3:D:1191:PRO:C	3:D:1193:THR:N	2.67	0.47
3:M:877:PRO:C	3:M:879:ARG:N	2.68	0.47
3:M:1060:SER:C	3:M:1062:ARG:N	2.67	0.47
3:M:1448:THR:C	3:M:1450:ALA:N	2.67	0.47
4:E:43:GLU:C	4:E:45:ARG:N	2.67	0.47
4:E:43:GLU:C	4:E:45:ARG:H	2.18	0.47
1:K:172:SER:C	1:K:174:VAL:H	2.17	0.47
3:D:1321:ALA:C	3:D:1323:GLN:H	2.16	0.47
2:L:342:ASP:C	2:L:344:PHE:H	2.18	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:583:LEU:C	2:L:585:GLU:N	2.68	0.47
2:C:582:GLY:C	2:C:584:GLU:N	2.68	0.47
3:D:102:ILE:C	3:D:104:PHE:N	2.64	0.47
3:D:100:ALA:C	3:D:102:ILE:H	2.18	0.47
1:J:122:ILE:C	1:J:124:ASN:H	2.18	0.47
2:C:272:ALA:C	2:C:274:ARG:N	2.67	0.47
3:M:734:GLU:C	3:M:736:PHE:N	2.68	0.47
3:D:877:PRO:C	3:D:879:ARG:N	2.68	0.46
3:D:989:TYR:C	3:D:991:GLN:N	2.66	0.46
4:N:43:GLU:C	4:N:45:ARG:N	2.68	0.46
2:C:342:ASP:C	2:C:344:PHE:H	2.18	0.46
3:D:734:GLU:C	3:D:736:PHE:N	2.68	0.46
5:H:270:ALA:C	5:H:272:THR:N	2.69	0.46
1:K:223:ASN:C	1:K:225:PHE:N	2.68	0.46
2:L:1083:GLU:C	2:L:1085:PHE:N	2.66	0.46
2:L:27:LYS:C	2:L:29:ALA:N	2.67	0.46
3:M:1220:ALA:C	3:M:1222:GLY:N	2.68	0.46
1:B:223:ASN:C	1:B:225:PHE:N	2.68	0.46
2:C:1001:VAL:C	2:C:1003:ASP:N	2.68	0.46
5:H:378:GLU:C	5:H:380:GLU:H	2.19	0.46
2:L:1001:VAL:C	2:L:1003:ASP:N	2.68	0.46
3:M:1321:ALA:C	3:M:1323:GLN:H	2.16	0.46
3:M:841:PHE:C	3:M:843:PHE:H	2.19	0.46
3:D:150:ARG:C	3:D:152:LEU:H	2.19	0.46
5:Q:179:LYS:C	5:Q:181:LEU:H	2.19	0.46
5:Q:270:ALA:C	5:Q:272:THR:N	2.69	0.46
3:M:148:GLU:C	3:M:150:ARG:H	2.18	0.46
5:Q:216:LYS:C	5:Q:218:THR:H	2.19	0.46
2:C:342:ASP:C	2:C:344:PHE:N	2.70	0.46
2:C:583:LEU:C	2:C:585:GLU:N	2.68	0.46
3:D:1226:ALA:C	3:D:1228:SER:N	2.68	0.46
3:D:148:GLU:C	3:D:150:ARG:H	2.18	0.46
5:H:216:LYS:C	5:H:218:THR:H	2.19	0.46
3:M:580:ALA:C	3:M:582:ILE:N	2.69	0.46
5:Q:421:ARG:C	5:Q:423:LEU:H	2.19	0.46
2:C:1083:GLU:C	2:C:1085:PHE:N	2.66	0.46
3:D:117:ASP:C	3:D:119:SER:N	2.70	0.46
1:J:118:ALA:C	1:J:120:VAL:H	2.20	0.46
2:L:272:ALA:C	2:L:274:ARG:N	2.67	0.46
3:M:150:ARG:C	3:M:152:LEU:H	2.19	0.46
3:M:487:ALA:C	3:M:489:ARG:N	2.70	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:508:ARG:C	3:M:510:GLU:H	2.19	0.46
3:M:688:TRP:C	3:M:690:ALA:N	2.69	0.46
3:D:1090:ASP:C	3:D:1092:GLY:N	2.69	0.45
3:D:580:ALA:C	3:D:582:ILE:N	2.69	0.45
4:N:43:GLU:C	4:N:45:ARG:H	2.18	0.45
5:Q:378:GLU:C	5:Q:380:GLU:H	2.19	0.45
3:D:508:ARG:C	3:D:510:GLU:H	2.19	0.45
3:D:841:PHE:C	3:D:843:PHE:H	2.19	0.45
2:L:437:ARG:C	2:L:439:CYS:N	2.69	0.45
2:L:976:ASP:C	2:L:978:ARG:H	2.19	0.45
3:D:1060:SER:C	3:D:1062:ARG:N	2.67	0.45
3:D:740:PHE:C	3:D:742:GLY:H	2.20	0.45
3:D:688:TRP:C	3:D:690:ALA:N	2.69	0.45
3:D:930:LEU:C	3:D:932:ASP:N	2.69	0.45
5:H:179:LYS:C	5:H:181:LEU:H	2.19	0.45
5:H:421:ARG:C	5:H:423:LEU:H	2.19	0.45
1:J:111:ALA:C	1:J:113:ASP:H	2.20	0.45
1:J:156:HIS:C	1:J:158:ILE:H	2.20	0.45
2:L:774:LEU:C	2:L:776:SER:H	2.20	0.45
3:M:740:PHE:C	3:M:742:GLY:H	2.20	0.45
3:M:892:ASP:C	3:M:894:LYS:N	2.70	0.45
2:C:1033:GLY:HA2	3:D:620:GLY:CA	2.37	0.45
3:D:619:LEU:C	3:D:621:LYS:H	2.20	0.45
4:E:84:ARG:C	4:E:86:GLN:N	2.70	0.45
2:L:342:ASP:C	2:L:344:PHE:N	2.70	0.45
3:M:1141:GLU:C	3:M:1143:GLY:N	2.68	0.45
1:A:111:ALA:C	1:A:113:ASP:H	2.20	0.45
3:D:1196:THR:C	3:D:1198:TYR:N	2.70	0.45
3:D:487:ALA:C	3:D:489:ARG:N	2.70	0.45
2:C:63:GLY:HA3	2:C:102:HIS:CA	2.47	0.45
4:E:86:GLN:C	4:E:89:MET:H	2.20	0.45
1:K:34:VAL:C	1:K:36:LEU:H	2.21	0.45
4:N:86:GLN:C	4:N:89:MET:H	2.20	0.45
3:M:1260:ILE:C	3:M:1262:LEU:N	2.68	0.45
3:M:619:LEU:C	3:M:621:LYS:H	2.20	0.45
1:B:79:ILE:C	1:B:81:ASN:N	2.70	0.44
2:C:178:ALA:C	2:C:180:GLY:N	2.70	0.44
2:C:450:GLY:C	2:C:452:ILE:N	2.70	0.44
2:C:976:ASP:C	2:C:978:ARG:H	2.19	0.44
3:D:470:LEU:C	3:D:472:LYS:N	2.71	0.44
3:D:892:ASP:C	3:D:894:LYS:N	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:63:GLY:HA3	2:L:102:HIS:CA	2.47	0.44
3:M:117:ASP:C	3:M:119:SER:N	2.69	0.44
3:M:1462:LEU:C	3:M:1464:GLU:N	2.69	0.44
3:D:1260:ILE:C	3:D:1262:LEU:N	2.68	0.44
3:M:470:LEU:C	3:M:472:LYS:N	2.71	0.44
1:A:156:HIS:C	1:A:158:ILE:H	2.20	0.44
2:C:774:LEU:C	2:C:776:SER:H	2.20	0.44
3:D:710:ARG:C	3:D:712:GLY:N	2.65	0.44
2:L:450:GLY:C	2:L:452:ILE:N	2.70	0.44
3:M:1090:ASP:C	3:M:1092:GLY:N	2.69	0.44
3:M:937:TYR:C	3:M:939:PHE:N	2.70	0.44
5:Q:211:VAL:C	5:Q:213:ILE:H	2.20	0.44
3:D:639:LEU:C	3:D:641:GLN:N	2.71	0.44
5:H:276:PRO:C	5:H:278:HIS:N	2.65	0.44
3:M:639:LEU:C	3:M:641:GLN:N	2.71	0.44
5:Q:179:LYS:C	5:Q:181:LEU:N	2.71	0.44
2:C:1041:GLU:C	2:C:1043:TYR:H	2.21	0.44
3:D:1220:ALA:C	3:D:1222:GLY:N	2.68	0.44
5:H:211:VAL:C	5:H:213:ILE:H	2.20	0.44
1:K:79:ILE:C	1:K:81:ASN:N	2.70	0.44
2:C:325:ILE:C	2:C:327:HIS:N	2.71	0.44
3:D:1172:HIS:C	3:D:1174:LEU:N	2.70	0.44
3:D:1448:THR:C	3:D:1450:ALA:N	2.67	0.44
2:L:20:GLU:C	2:L:22:GLN:N	2.71	0.44
3:M:1191:PRO:C	3:M:1193:THR:N	2.67	0.44
3:D:1321:ALA:C	3:D:1323:GLN:N	2.71	0.44
2:C:692:GLU:C	2:C:694:LEU:N	2.70	0.44
3:D:815:ALA:C	3:D:817:GLU:H	2.21	0.44
3:M:930:LEU:C	3:M:932:ASP:N	2.69	0.44
1:B:34:VAL:C	1:B:36:LEU:H	2.21	0.43
5:H:179:LYS:C	5:H:181:LEU:N	2.71	0.43
1:K:70:GLY:HA3	1:K:135:GLY:HA3	2.00	0.43
3:M:1196:THR:C	3:M:1198:TYR:N	2.70	0.43
3:M:996:TRP:C	3:M:998:GLU:N	2.69	0.43
2:L:919:ALA:C	2:L:921:ALA:H	2.21	0.43
4:N:84:ARG:C	4:N:86:GLN:N	2.70	0.43
2:C:965:GLU:C	2:C:967:PHE:N	2.71	0.43
3:D:757:ALA:C	3:D:759:ALA:N	2.70	0.43
3:D:993:ILE:C	3:D:995:LEU:N	2.71	0.43
2:L:1041:GLU:C	2:L:1043:TYR:H	2.21	0.43
2:L:430:VAL:C	2:L:432:ARG:N	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:ALA:C	1:A:120:VAL:H	2.20	0.43
3:D:855:HIS:C	3:D:857:LEU:N	2.70	0.43
2:L:946:ARG:C	2:L:948:GLU:N	2.71	0.43
3:M:22:SER:C	3:M:24:GLY:H	2.22	0.43
3:M:815:ALA:C	3:M:817:GLU:H	2.21	0.43
2:L:582:GLY:C	2:L:584:GLU:N	2.68	0.43
4:N:11:GLY:C	4:N:13:VAL:N	2.71	0.43
2:C:561:GLY:C	2:C:563:ASN:N	2.71	0.43
3:M:1386:ASP:C	3:M:1388:ARG:H	2.22	0.43
2:C:20:GLU:C	2:C:22:GLN:N	2.71	0.43
3:D:22:SER:C	3:D:24:GLY:H	2.22	0.43
3:M:1172:HIS:C	3:M:1174:LEU:N	2.70	0.43
3:M:602:SER:C	3:M:604:THR:H	2.22	0.43
2:C:583:LEU:C	2:C:585:GLU:H	2.21	0.43
2:C:919:ALA:C	2:C:921:ALA:H	2.21	0.43
4:N:70:THR:C	4:N:72:ARG:N	2.69	0.43
3:D:1386:ASP:C	3:D:1388:ARG:H	2.22	0.43
1:B:70:GLY:HA3	1:B:135:GLY:HA3	2.00	0.43
3:D:1462:LEU:C	3:D:1464:GLU:N	2.69	0.43
3:D:937:TYR:C	3:D:939:PHE:N	2.70	0.43
4:E:70:THR:C	4:E:72:ARG:N	2.69	0.43
4:E:83:ASP:C	4:E:85:LEU:H	2.22	0.43
2:C:946:ARG:C	2:C:948:GLU:N	2.71	0.42
1:J:71:VAL:C	2:L:608:GLY:HA2	2.40	0.42
2:L:692:GLU:C	2:L:694:LEU:N	2.70	0.42
3:M:1321:ALA:C	3:M:1323:GLN:N	2.71	0.42
3:M:731:LEU:C	3:M:733:CYS:N	2.70	0.42
2:L:178:ALA:C	2:L:180:GLY:N	2.70	0.42
2:L:917:LEU:C	2:L:919:ALA:N	2.73	0.42
3:M:643:GLY:HA3	3:M:727:GLN:N	2.33	0.42
3:D:731:LEU:C	3:D:733:CYS:N	2.70	0.42
3:M:764:LEU:C	3:M:766:ALA:N	2.73	0.42
3:M:937:TYR:C	3:M:939:PHE:H	2.23	0.42
3:M:467:GLU:C	3:M:469:ASP:N	2.73	0.42
1:A:189:ARG:C	1:A:191:ASP:H	2.22	0.42
2:C:302:VAL:C	2:C:304:LEU:N	2.73	0.42
2:L:570:PRO:C	2:L:572:ILE:N	2.72	0.42
3:M:1098:LEU:C	3:M:1100:ASP:N	2.72	0.42
3:D:996:TRP:C	3:D:998:GLU:N	2.69	0.42
1:J:79:ILE:C	1:J:81:ASN:N	2.72	0.42
3:M:1009:LYS:C	3:M:1011:PHE:N	2.70	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:937:TYR:C	3:D:939:PHE:H	2.23	0.42
2:L:549:PHE:C	2:L:551:GLU:N	2.72	0.42
3:M:855:HIS:C	3:M:857:LEU:N	2.70	0.42
1:A:71:VAL:C	2:C:608:GLY:HA2	2.40	0.42
2:C:320:HIS:C	2:C:322:VAL:H	2.23	0.42
2:C:917:LEU:C	2:C:919:ALA:N	2.73	0.42
4:E:17:TYR:C	4:E:19:LEU:N	2.72	0.42
2:L:583:LEU:C	2:L:585:GLU:H	2.21	0.42
3:M:885:ILE:C	3:M:887:GLY:N	2.73	0.42
3:D:1098:LEU:C	3:D:1100:ASP:N	2.72	0.42
4:E:67:GLU:C	4:E:69:LEU:H	2.24	0.42
2:L:1015:LEU:C	2:L:1017:THR:N	2.73	0.42
2:L:965:GLU:C	2:L:967:PHE:N	2.71	0.42
4:N:17:TYR:C	4:N:19:LEU:N	2.72	0.42
4:N:67:GLU:C	4:N:69:LEU:H	2.24	0.42
2:C:437:ARG:C	2:C:439:CYS:N	2.69	0.42
1:J:189:ARG:C	1:J:191:ASP:H	2.22	0.42
3:M:993:ILE:C	3:M:995:LEU:N	2.71	0.42
4:N:83:ASP:C	4:N:85:LEU:H	2.22	0.42
1:A:79:ILE:C	1:A:81:ASN:N	2.72	0.41
2:C:1001:VAL:C	2:C:1003:ASP:H	2.23	0.41
4:E:11:GLY:C	4:E:13:VAL:N	2.71	0.41
3:D:602:SER:C	3:D:604:THR:H	2.22	0.41
3:D:764:LEU:C	3:D:766:ALA:H	2.24	0.41
3:D:764:LEU:C	3:D:766:ALA:N	2.72	0.41
3:D:885:ILE:C	3:D:887:GLY:N	2.73	0.41
3:D:941:LEU:C	3:D:943:THR:N	2.71	0.41
2:L:1001:VAL:C	2:L:1003:ASP:H	2.23	0.41
3:M:491:LYS:C	3:M:493:ARG:N	2.73	0.41
4:N:84:ARG:C	4:N:87:LYS:H	2.24	0.41
2:C:663:GLU:C	2:C:665:PHE:H	2.24	0.41
3:D:82:ARG:C	3:D:84:ILE:H	2.23	0.41
2:L:171:TRP:H	2:L:187:ASN:CA	2.33	0.41
2:L:320:HIS:C	2:L:322:VAL:H	2.23	0.41
2:C:549:PHE:C	2:C:551:GLU:N	2.72	0.41
2:L:463:ALA:C	2:L:465:GLY:N	2.72	0.41
3:M:1090:ASP:C	3:M:1092:GLY:H	2.23	0.41
3:M:1353:GLN:C	3:M:1355:VAL:N	2.74	0.41
2:C:1015:LEU:C	2:C:1017:THR:N	2.73	0.41
2:L:347:GLY:C	2:L:349:ALA:N	2.70	0.41
2:L:808:ARG:C	2:L:810:ASP:N	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:56:TYR:C	3:M:58:CYS:H	2.24	0.41
2:C:430:VAL:C	2:C:432:ARG:N	2.72	0.41
3:D:1129:THR:C	3:D:1131:THR:H	2.24	0.41
3:D:1270:ALA:C	3:D:1272:ALA:H	2.23	0.41
3:D:465:LEU:C	3:D:467:GLU:N	2.72	0.41
2:L:325:ILE:C	2:L:327:HIS:N	2.71	0.41
3:M:21:TRP:C	3:M:23:TYR:N	2.73	0.41
2:C:463:ALA:C	2:C:465:GLY:N	2.72	0.41
3:D:1331:ASP:C	3:D:1333:HIS:H	2.24	0.41
3:M:1270:ALA:C	3:M:1272:ALA:H	2.23	0.41
3:M:541:ASN:C	3:M:543:LEU:H	2.24	0.41
3:D:1020:LEU:C	3:D:1022:VAL:N	2.74	0.41
3:D:1090:ASP:C	3:D:1092:GLY:H	2.23	0.41
3:D:56:TYR:C	3:D:58:CYS:H	2.24	0.41
3:M:1129:THR:C	3:M:1131:THR:H	2.24	0.41
3:D:541:ASN:C	3:D:543:LEU:H	2.24	0.41
2:L:943:VAL:C	2:L:945:ALA:H	2.24	0.41
3:M:82:ARG:C	3:M:84:ILE:H	2.23	0.41
2:L:302:VAL:C	2:L:304:LEU:N	2.73	0.41
3:M:941:LEU:C	3:M:943:THR:N	2.71	0.41
2:C:884:GLN:C	2:C:886:LEU:N	2.75	0.41
3:D:643:GLY:HA3	3:D:727:GLN:N	2.33	0.41
2:L:561:GLY:C	2:L:563:ASN:N	2.71	0.41
3:M:1032:PRO:C	3:M:1034:GLN:N	2.74	0.41
5:Q:94:ASP:C	5:Q:96:VAL:H	2.25	0.41
2:C:520:GLU:C	2:C:522:VAL:N	2.75	0.40
2:C:570:PRO:C	2:C:572:ILE:N	2.72	0.40
4:N:57:ASP:C	4:N:59:ASN:H	2.25	0.40
1:B:172:SER:C	1:B:174:VAL:N	2.75	0.40
3:D:1100:ASP:C	3:D:1102:ALA:N	2.75	0.40
3:D:31:THR:C	3:D:33:ASN:H	2.25	0.40
4:E:84:ARG:C	4:E:87:LYS:H	2.24	0.40
2:L:1055:ILE:C	2:L:1057:SER:H	2.25	0.40
3:M:31:THR:C	3:M:33:ASN:H	2.25	0.40
2:C:915:LYS:C	2:C:917:LEU:N	2.73	0.40
3:D:1353:GLN:C	3:D:1355:VAL:N	2.74	0.40
3:D:138:LYS:C	3:D:140:ALA:H	2.25	0.40
3:D:571:LYS:C	3:D:573:MET:N	2.74	0.40
2:L:663:GLU:C	2:L:665:PHE:H	2.24	0.40
3:M:571:LYS:C	3:M:573:MET:N	2.74	0.40
5:H:94:ASP:C	5:H:96:VAL:H	2.25	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:1331:ASP:C	3:M:1333:HIS:H	2.24	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	222/314 (71%)	95 (43%)	65 (29%)	62 (28%)	0	0
1	B	218/314 (69%)	110 (50%)	53 (24%)	55 (25%)	0	1
1	J	222/314 (71%)	95 (43%)	65 (29%)	62 (28%)	0	0
1	K	218/314 (69%)	110 (50%)	53 (24%)	55 (25%)	0	1
2	C	1072/1118 (96%)	439 (41%)	296 (28%)	337 (31%)	0	0
2	L	1072/1118 (96%)	439 (41%)	294 (27%)	339 (32%)	0	0
3	D	1175/1524 (77%)	456 (39%)	307 (26%)	412 (35%)	0	0
3	M	1175/1524 (77%)	456 (39%)	309 (26%)	410 (35%)	0	0
4	E	90/99 (91%)	40 (44%)	24 (27%)	26 (29%)	0	0
4	N	90/99 (91%)	40 (44%)	24 (27%)	26 (29%)	0	0
5	H	318/332 (96%)	209 (66%)	57 (18%)	52 (16%)	0	3
5	Q	318/332 (96%)	209 (66%)	57 (18%)	52 (16%)	0	3
All	All	6190/7402 (84%)	2698 (44%)	1604 (26%)	1888 (30%)	0	0

All (1888) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	59	GLU
1	A	64	GLU
1	A	76	VAL

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Mol	Chain	Res	Type
1	A	125	PRO
1	A	137	LYS
1	A	148	VAL
1	A	153	ALA
1	A	158	ILE
1	A	162	ILE
1	A	172	SER
1	A	176	ARG
1	A	182	GLU
1	A	188	GLN
1	A	199	ILE
1	A	208	LEU
1	A	216	ALA
1	A	226	ALA
1	B	7	LYS
1	B	15	THR
1	B	29	GLU
1	B	54	THR
1	B	75	VAL
1	B	91	ASP
1	B	104	GLU
1	B	106	PRO
1	B	114	PHE
1	B	128	HIS
1	B	135	GLY
1	B	158	ILE
1	B	171	PHE
1	B	181	VAL
1	B	185	ARG
1	B	186	LEU
1	B	191	ASP
1	B	195	LEU
1	B	200	TRP
1	B	224	TYR
2	C	17	PRO
2	C	22	GLN
2	C	27	LYS
2	C	31	GLN
2	C	33	ASP
2	C	40	GLU
2	C	42	VAL
2	C	46	ALA

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Mol	Chain	Res	Type
2	C	47	ALA
2	C	54	ILE
2	C	70	GLU
2	C	80	GLN
2	C	88	LEU
2	C	102	HIS
2	C	109	LYS
2	C	111	ASP
2	C	114	PHE
2	C	115	LEU
2	C	136	ILE
2	C	137	VAL
2	C	153	ALA
2	C	155	PRO
2	C	168	ARG
2	C	182	VAL
2	C	187	ASN
2	C	199	VAL
2	C	221	LEU
2	C	244	PRO
2	C	263	ASP
2	C	264	PRO
2	C	269	LEU
2	C	275	TYR
2	C	278	GLU
2	C	288	ARG
2	C	322	VAL
2	C	336	VAL
2	C	370	ALA
2	C	392	SER
2	C	395	LYS
2	C	397	GLU
2	C	398	THR
2	C	402	SER
2	C	409	ARG
2	C	418	LEU
2	C	420	ARG
2	C	425	PHE
2	C	430	VAL
2	C	431	HIS
2	C	432	ARG
2	C	434	HIS

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Mol	Chain	Res	Type
2	C	444	PRO
2	C	449	ILE
2	C	451	LEU
2	C	457	ALA
2	C	483	VAL
2	C	496	ILE
2	C	498	GLN
2	C	503	LEU
2	C	518	ARG
2	C	522	VAL
2	C	526	PRO
2	C	530	GLU
2	C	532	MET
2	C	537	LYS
2	C	541	SER
2	C	543	ASN
2	C	545	ASN
2	C	548	PRO
2	C	574	ALA
2	C	580	MET
2	C	587	VAL
2	C	588	VAL
2	C	599	GLU
2	C	603	VAL
2	C	604	VAL
2	C	612	ALA
2	C	616	GLU
2	C	629	ALA
2	C	633	GLN
2	C	641	PRO
2	C	643	VAL
2	C	644	ARG
2	C	656	ALA
2	C	657	ASP
2	C	663	GLU
2	C	677	MET
2	C	713	ARG
2	C	714	ASP
2	C	715	THR
2	C	728	HIS
2	C	735	ARG
2	C	738	ASP

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Mol	Chain	Res	Type
2	C	760	SER
2	C	762	LYS
2	C	767	PRO
2	C	788	THR
2	C	804	LEU
2	C	831	ARG
2	C	832	LYS
2	C	840	ALA
2	C	848	VAL
2	C	849	VAL
2	C	871	LEU
2	C	880	MET
2	C	884	GLN
2	C	885	ILE
2	C	919	ALA
2	C	920	GLU
2	C	944	LEU
2	C	957	LYS
2	C	964	LYS
2	C	965	GLU
2	C	967	PHE
2	C	973	VAL
2	C	974	LEU
2	C	984	GLU
2	C	999	HIS
2	C	1000	MET
2	C	1011	GLY
2	C	1012	PRO
2	C	1021	LEU
2	C	1027	PHE
2	C	1035	MET
2	C	1038	TRP
2	C	1053	LEU
2	C	1075	ASP
2	C	1078	GLU
2	C	1104	GLU
3	D	5	VAL
3	D	10	ILE
3	D	12	LEU
3	D	13	ALA
3	D	26	VAL
3	D	28	LYS

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Mol	Chain	Res	Type
3	D	33	ASN
3	D	41	ARG
3	D	52	PRO
3	D	64	LYS
3	D	97	THR
3	D	98	PRO
3	D	100	ALA
3	D	109	PRO
3	D	110	SER
3	D	117	ASP
3	D	119	SER
3	D	126	VAL
3	D	131	LYS
3	D	140	ALA
3	D	141	VAL
3	D	143	ASP
3	D	146	PRO
3	D	147	VAL
3	D	454	ALA
3	D	477	LEU
3	D	478	LEU
3	D	479	GLU
3	D	484	PRO
3	D	486	ARG
3	D	487	ALA
3	D	488	ARG
3	D	491	LYS
3	D	526	PRO
3	D	530	VAL
3	D	531	ASP
3	D	535	PHE
3	D	547	LEU
3	D	548	ILE
3	D	564	GLU
3	D	565	ILE
3	D	571	LYS
3	D	582	ILE
3	D	607	LEU
3	D	626	SER
3	D	630	VAL
3	D	633	VAL
3	D	638	LYS

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Mol	Chain	Res	Type
3	D	646	LYS
3	D	647	ARG
3	D	648	MET
3	D	649	ALA
3	D	650	LEU
3	D	655	PRO
3	D	662	GLU
3	D	665	ALA
3	D	668	PRO
3	D	672	ALA
3	D	678	GLU
3	D	679	ARG
3	D	682	ASP
3	D	684	LYS
3	D	696	HIS
3	D	702	LEU
3	D	718	PRO
3	D	725	SER
3	D	730	PRO
3	D	731	LEU
3	D	739	ASP
3	D	762	GLN
3	D	770	LEU
3	D	782	SER
3	D	793	THR
3	D	795	VAL
3	D	797	LYS
3	D	799	LYS
3	D	807	ALA
3	D	808	THR
3	D	811	GLU
3	D	815	ALA
3	D	821	VAL
3	D	825	ALA
3	D	826	PRO
3	D	828	VAL
3	D	829	VAL
3	D	835	SER
3	D	838	ARG
3	D	840	LYS
3	D	842	VAL
3	D	848	GLU

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Mol	Chain	Res	Type
3	D	849	ALA
3	D	862	ASP
3	D	875	THR
3	D	898	GLU
3	D	899	LEU
3	D	900	ILE
3	D	905	PRO
3	D	908	LYS
3	D	919	PHE
3	D	924	MET
3	D	925	GLU
3	D	947	ILE
3	D	948	THR
3	D	953	ASP
3	D	961	GLN
3	D	966	GLU
3	D	1000	THR
3	D	1006	ALA
3	D	1016	PRO
3	D	1023	MET
3	D	1028	ALA
3	D	1029	ARG
3	D	1040	GLY
3	D	1045	MET
3	D	1054	GLU
3	D	1059	SER
3	D	1061	PHE
3	D	1067	VAL
3	D	1109	GLU
3	D	1111	ASP
3	D	1113	GLY
3	D	1116	ASN
3	D	1141	GLU
3	D	1149	LEU
3	D	1152	GLU
3	D	1178	ALA
3	D	1190	SER
3	D	1194	CYS
3	D	1195	GLN
3	D	1201	CYS
3	D	1203	LYS
3	D	1208	ASP

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Mol	Chain	Res	Type
3	D	1209	LEU
3	D	1210	SER
3	D	1219	GLU
3	D	1223	VAL
3	D	1224	VAL
3	D	1225	ALA
3	D	1231	GLU
3	D	1232	PRO
3	D	1234	THR
3	D	1236	LEU
3	D	1239	ARG
3	D	1268	PRO
3	D	1276	GLU
3	D	1281	VAL
3	D	1296	SER
3	D	1300	SER
3	D	1306	PRO
3	D	1313	VAL
3	D	1320	GLU
3	D	1321	ALA
3	D	1323	GLN
3	D	1330	ILE
3	D	1347	TYR
3	D	1364	HIS
3	D	1366	LYS
3	D	1367	HIS
3	D	1373	ARG
3	D	1374	GLN
3	D	1375	MET
3	D	1384	PRO
3	D	1388	ARG
3	D	1394	VAL
3	D	1396	GLU
3	D	1408	ILE
3	D	1424	VAL
3	D	1436	SER
3	D	1439	SER
3	D	1442	ASN
3	D	1445	HIS
3	D	1448	THR
3	D	1451	ALA
3	D	1452	ILE

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Mol	Chain	Res	Type
3	D	1455	LYS
3	D	1457	ASP
3	D	1458	GLU
3	D	1462	LEU
3	D	1464	GLU
3	D	1483	PHE
3	D	1487	VAL
4	E	16	LYS
4	E	21	VAL
4	E	30	LEU
4	E	34	ARG
4	E	42	PRO
4	E	50	THR
4	E	51	LEU
4	E	60	ALA
4	E	61	VAL
4	E	77	GLU
4	E	90	GLU
5	H	171	VAL
5	H	203	ILE
5	H	211	VAL
5	H	220	ARG
5	H	249	LYS
5	H	251	SER
5	H	328	GLU
5	H	329	PRO
5	H	333	GLU
5	H	335	PRO
5	H	352	ASN
5	H	407	VAL
5	H	409	ARG
5	H	420	LEU
5	H	432	LYS
1	J	59	GLU
1	J	64	GLU
1	J	76	VAL
1	J	125	PRO
1	J	137	LYS
1	J	148	VAL
1	J	153	ALA
1	J	158	ILE
1	J	162	ILE

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Mol	Chain	Res	Type
1	J	172	SER
1	J	176	ARG
1	J	182	GLU
1	J	188	GLN
1	J	199	ILE
1	J	208	LEU
1	J	216	ALA
1	J	226	ALA
1	K	7	LYS
1	K	15	THR
1	K	29	GLU
1	K	54	THR
1	K	75	VAL
1	K	91	ASP
1	K	104	GLU
1	K	106	PRO
1	K	114	PHE
1	K	128	HIS
1	K	135	GLY
1	K	158	ILE
1	K	171	PHE
1	K	181	VAL
1	K	185	ARG
1	K	186	LEU
1	K	191	ASP
1	K	195	LEU
1	K	200	TRP
1	K	224	TYR
2	L	17	PRO
2	L	22	GLN
2	L	27	LYS
2	L	31	GLN
2	L	33	ASP
2	L	40	GLU
2	L	42	VAL
2	L	46	ALA
2	L	47	ALA
2	L	54	ILE
2	L	70	GLU
2	L	80	GLN
2	L	88	LEU
2	L	102	HIS

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Mol	Chain	Res	Type
2	L	109	LYS
2	L	111	ASP
2	L	114	PHE
2	L	115	LEU
2	L	136	ILE
2	L	137	VAL
2	L	153	ALA
2	L	155	PRO
2	L	168	ARG
2	L	182	VAL
2	L	187	ASN
2	L	199	VAL
2	L	221	LEU
2	L	244	PRO
2	L	263	ASP
2	L	264	PRO
2	L	269	LEU
2	L	275	TYR
2	L	278	GLU
2	L	288	ARG
2	L	322	VAL
2	L	336	VAL
2	L	370	ALA
2	L	392	SER
2	L	395	LYS
2	L	397	GLU
2	L	398	THR
2	L	402	SER
2	L	409	ARG
2	L	418	LEU
2	L	420	ARG
2	L	425	PHE
2	L	430	VAL
2	L	431	HIS
2	L	432	ARG
2	L	434	HIS
2	L	444	PRO
2	L	449	ILE
2	L	451	LEU
2	L	457	ALA
2	L	483	VAL
2	L	496	ILE

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Mol	Chain	Res	Type
2	L	498	GLN
2	L	503	LEU
2	L	518	ARG
2	L	522	VAL
2	L	526	PRO
2	L	530	GLU
2	L	532	MET
2	L	537	LYS
2	L	541	SER
2	L	543	ASN
2	L	545	ASN
2	L	548	PRO
2	L	574	ALA
2	L	580	MET
2	L	587	VAL
2	L	588	VAL
2	L	599	GLU
2	L	603	VAL
2	L	604	VAL
2	L	612	ALA
2	L	616	GLU
2	L	629	ALA
2	L	633	GLN
2	L	641	PRO
2	L	643	VAL
2	L	644	ARG
2	L	656	ALA
2	L	657	ASP
2	L	663	GLU
2	L	677	MET
2	L	713	ARG
2	L	714	ASP
2	L	715	THR
2	L	728	HIS
2	L	735	ARG
2	L	738	ASP
2	L	760	SER
2	L	762	LYS
2	L	767	PRO
2	L	788	THR
2	L	804	LEU
2	L	831	ARG

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Mol	Chain	Res	Type
2	L	832	LYS
2	L	840	ALA
2	L	848	VAL
2	L	849	VAL
2	L	871	LEU
2	L	880	MET
2	L	884	GLN
2	L	885	ILE
2	L	919	ALA
2	L	920	GLU
2	L	944	LEU
2	L	957	LYS
2	L	964	LYS
2	L	965	GLU
2	L	967	PHE
2	L	973	VAL
2	L	974	LEU
2	L	984	GLU
2	L	999	HIS
2	L	1000	MET
2	L	1011	GLY
2	L	1012	PRO
2	L	1021	LEU
2	L	1027	PHE
2	L	1035	MET
2	L	1038	TRP
2	L	1053	LEU
2	L	1075	ASP
2	L	1078	GLU
2	L	1104	GLU
3	M	5	VAL
3	M	10	ILE
3	M	12	LEU
3	M	13	ALA
3	M	26	VAL
3	M	28	LYS
3	M	33	ASN
3	M	41	ARG
3	M	52	PRO
3	M	64	LYS
3	M	97	THR
3	M	98	PRO

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Mol	Chain	Res	Type
3	M	100	ALA
3	M	109	PRO
3	M	110	SER
3	M	117	ASP
3	M	119	SER
3	M	126	VAL
3	M	131	LYS
3	M	140	ALA
3	M	141	VAL
3	M	143	ASP
3	M	146	PRO
3	M	147	VAL
3	M	454	ALA
3	M	477	LEU
3	M	478	LEU
3	M	479	GLU
3	M	484	PRO
3	M	486	ARG
3	M	487	ALA
3	M	488	ARG
3	M	491	LYS
3	M	526	PRO
3	M	530	VAL
3	M	531	ASP
3	M	535	PHE
3	M	547	LEU
3	M	548	ILE
3	M	564	GLU
3	M	565	ILE
3	M	571	LYS
3	M	582	ILE
3	M	607	LEU
3	M	626	SER
3	M	630	VAL
3	M	633	VAL
3	M	638	LYS
3	M	646	LYS
3	M	647	ARG
3	M	648	MET
3	M	649	ALA
3	M	650	LEU
3	M	655	PRO

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Mol	Chain	Res	Type
3	M	662	GLU
3	M	665	ALA
3	M	668	PRO
3	M	672	ALA
3	M	678	GLU
3	M	679	ARG
3	M	682	ASP
3	M	684	LYS
3	M	696	HIS
3	M	702	LEU
3	M	718	PRO
3	M	725	SER
3	M	730	PRO
3	M	731	LEU
3	M	739	ASP
3	M	762	GLN
3	M	770	LEU
3	M	782	SER
3	M	793	THR
3	M	795	VAL
3	M	797	LYS
3	M	799	LYS
3	M	807	ALA
3	M	808	THR
3	M	811	GLU
3	M	815	ALA
3	M	821	VAL
3	M	825	ALA
3	M	826	PRO
3	M	828	VAL
3	M	829	VAL
3	M	835	SER
3	M	838	ARG
3	M	840	LYS
3	M	842	VAL
3	M	848	GLU
3	M	849	ALA
3	M	862	ASP
3	M	875	THR
3	M	898	GLU
3	M	899	LEU
3	M	900	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	M	905	PRO
3	M	908	LYS
3	M	919	PHE
3	M	924	MET
3	M	925	GLU
3	M	947	ILE
3	M	948	THR
3	M	953	ASP
3	M	961	GLN
3	M	966	GLU
3	M	1000	THR
3	M	1006	ALA
3	M	1016	PRO
3	M	1023	MET
3	M	1028	ALA
3	M	1029	ARG
3	M	1040	GLY
3	M	1045	MET
3	M	1054	GLU
3	M	1059	SER
3	M	1061	PHE
3	M	1067	VAL
3	M	1109	GLU
3	M	1111	ASP
3	M	1113	GLY
3	M	1116	ASN
3	M	1141	GLU
3	M	1149	LEU
3	M	1152	GLU
3	M	1178	ALA
3	M	1190	SER
3	M	1194	CYS
3	M	1195	GLN
3	M	1201	CYS
3	M	1203	LYS
3	M	1208	ASP
3	M	1209	LEU
3	M	1210	SER
3	M	1219	GLU
3	M	1223	VAL
3	M	1224	VAL
3	M	1225	ALA

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Mol	Chain	Res	Type
3	M	1231	GLU
3	M	1232	PRO
3	M	1234	THR
3	M	1236	LEU
3	M	1239	ARG
3	M	1268	PRO
3	M	1276	GLU
3	M	1281	VAL
3	M	1296	SER
3	M	1300	SER
3	M	1306	PRO
3	M	1313	VAL
3	M	1320	GLU
3	M	1321	ALA
3	M	1323	GLN
3	M	1330	ILE
3	M	1347	TYR
3	M	1364	HIS
3	M	1366	LYS
3	M	1367	HIS
3	M	1373	ARG
3	M	1374	GLN
3	M	1375	MET
3	M	1384	PRO
3	M	1388	ARG
3	M	1394	VAL
3	M	1396	GLU
3	M	1408	ILE
3	M	1424	VAL
3	M	1436	SER
3	M	1439	SER
3	M	1442	ASN
3	M	1445	HIS
3	M	1448	THR
3	M	1451	ALA
3	M	1452	ILE
3	M	1455	LYS
3	M	1457	ASP
3	M	1458	GLU
3	M	1462	LEU
3	M	1464	GLU
3	M	1483	PHE

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Mol	Chain	Res	Type
3	M	1487	VAL
4	N	16	LYS
4	N	21	VAL
4	N	30	LEU
4	N	34	ARG
4	N	42	PRO
4	N	50	THR
4	N	51	LEU
4	N	60	ALA
4	N	61	VAL
4	N	77	GLU
4	N	90	GLU
5	Q	171	VAL
5	Q	203	ILE
5	Q	211	VAL
5	Q	220	ARG
5	Q	249	LYS
5	Q	251	SER
5	Q	328	GLU
5	Q	329	PRO
5	Q	333	GLU
5	Q	335	PRO
5	Q	352	ASN
5	Q	407	VAL
5	Q	409	ARG
5	Q	420	LEU
5	Q	432	LYS
1	A	13	ALA
1	A	36	LEU
1	A	44	LEU
1	A	46	SER
1	A	54	THR
1	A	65	PHE
1	A	107	LYS
1	A	112	GLY
1	A	123	MET
1	A	126	ASP
1	A	132	LEU
1	A	138	LEU
1	A	164	ALA
1	A	189	ARG
1	A	209	GLU

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Mol	Chain	Res	Type
1	A	211	LEU
1	A	215	VAL
1	A	224	TYR
1	A	228	PRO
1	B	35	THR
1	B	53	VAL
1	B	70	GLY
1	B	78	ILE
1	B	112	GLY
1	B	117	SER
1	B	137	LYS
1	B	138	LEU
1	B	152	PRO
1	B	196	THR
1	B	201	THR
1	B	202	ASP
1	B	204	SER
1	B	208	LEU
2	C	24	GLU
2	C	28	LYS
2	C	43	GLY
2	C	81	ASP
2	C	108	ILE
2	C	112	GLU
2	C	133	ASP
2	C	144	PRO
2	C	157	ARG
2	C	177	GLU
2	C	179	SER
2	C	237	ARG
2	C	316	GLY
2	C	326	ASP
2	C	338	GLU
2	C	381	ALA
2	C	391	LEU
2	C	393	GLN
2	C	423	ALA
2	C	427	VAL
2	C	438	ILE
2	C	445	GLU
2	C	450	GLY
2	C	458	TYR

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Mol	Chain	Res	Type
2	C	460	ARG
2	C	489	SER
2	C	494	TYR
2	C	502	PRO
2	C	508	ILE
2	C	514	VAL
2	C	529	VAL
2	C	534	VAL
2	C	536	PRO
2	C	550	LEU
2	C	560	MET
2	C	582	GLY
2	C	589	ARG
2	C	600	ASP
2	C	605	LYS
2	C	608	GLY
2	C	620	LEU
2	C	635	THR
2	C	655	LEU
2	C	666	LEU
2	C	685	GLU
2	C	698	ASP
2	C	761	PHE
2	C	769	PRO
2	C	775	ARG
2	C	787	ASP
2	C	791	ARG
2	C	793	PRO
2	C	808	ARG
2	C	809	GLY
2	C	855	VAL
2	C	857	ASP
2	C	876	VAL
2	C	877	PRO
2	C	894	GLY
2	C	928	LYS
2	C	933	GLY
2	C	945	ALA
2	C	960	GLU
2	C	968	ASP
2	C	972	VAL
2	C	981	GLU

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Mol	Chain	Res	Type
2	C	987	ILE
2	C	1001	VAL
2	C	1037	VAL
2	C	1046	ALA
2	C	1056	LYS
2	C	1060	ILE
2	C	1066	ALA
2	C	1079	PRO
2	C	1082	PRO
2	C	1083	GLU
2	C	1093	GLN
2	C	1096	ALA
2	C	1106	ASP
2	C	1113	GLU
2	C	1114	GLY
3	D	7	LYS
3	D	14	SER
3	D	18	ILE
3	D	32	ILE
3	D	37	LEU
3	D	43	GLY
3	D	45	PHE
3	D	47	GLU
3	D	67	ARG
3	D	72	VAL
3	D	85	VAL
3	D	99	ALA
3	D	102	ILE
3	D	127	LEU
3	D	129	PHE
3	D	139	GLY
3	D	464	LEU
3	D	480	GLU
3	D	485	SER
3	D	498	VAL
3	D	502	PHE
3	D	506	GLY
3	D	540	LEU
3	D	545	ARG
3	D	558	LEU
3	D	567	ILE
3	D	586	ARG

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Mol	Chain	Res	Type
3	D	595	GLY
3	D	601	ARG
3	D	605	ASP
3	D	609	GLY
3	D	621	LYS
3	D	640	HIS
3	D	643	GLY
3	D	681	ARG
3	D	686	GLU
3	D	689	ASP
3	D	695	ILE
3	D	712	GLY
3	D	715	ALA
3	D	723	GLY
3	D	724	GLN
3	D	735	ALA
3	D	776	GLU
3	D	783	ARG
3	D	784	ASP
3	D	794	GLN
3	D	796	ARG
3	D	803	GLY
3	D	819	GLY
3	D	822	ALA
3	D	864	VAL
3	D	872	ARG
3	D	892	ASP
3	D	893	GLU
3	D	897	GLN
3	D	913	ASP
3	D	920	LEU
3	D	928	ALA
3	D	936	TYR
3	D	958	GLU
3	D	964	LEU
3	D	994	GLN
3	D	1001	GLU
3	D	1020	LEU
3	D	1042	ARG
3	D	1056	PRO
3	D	1070	TYR
3	D	1099	VAL

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Mol	Chain	Res	Type
3	D	1142	SER
3	D	1146	GLY
3	D	1173	PHE
3	D	1175	ILE
3	D	1179	GLU
3	D	1180	ALA
3	D	1188	VAL
3	D	1200	VAL
3	D	1212	ALA
3	D	1215	VAL
3	D	1233	GLY
3	D	1237	THR
3	D	1263	PHE
3	D	1273	VAL
3	D	1287	GLU
3	D	1328	GLY
3	D	1339	LYS
3	D	1353	GLN
3	D	1360	GLY
3	D	1361	VAL
3	D	1365	ASP
3	D	1381	VAL
3	D	1386	ASP
3	D	1397	LYS
3	D	1430	SER
3	D	1449	GLU
3	D	1454	GLY
3	D	1466	VAL
3	D	1473	PRO
3	D	1475	GLY
4	E	6	ILE
4	E	10	PHE
4	E	12	MET
4	E	15	SER
4	E	22	VAL
4	E	23	VAL
4	E	24	ALA
4	E	41	GLU
5	H	108	LEU
5	H	111	LEU
5	H	152	GLY
5	H	172	GLU

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Mol	Chain	Res	Type
5	H	173	GLU
5	H	176	GLY
5	H	186	LYS
5	H	277	VAL
5	H	315	ASP
5	H	331	SER
5	H	349	PRO
5	H	351	GLU
5	H	387	ARG
5	H	406	GLY
5	H	410	GLU
5	H	419	ALA
5	H	431	ARG
1	J	13	ALA
1	J	36	LEU
1	J	44	LEU
1	J	46	SER
1	J	54	THR
1	J	65	PHE
1	J	107	LYS
1	J	112	GLY
1	J	123	MET
1	J	126	ASP
1	J	132	LEU
1	J	138	LEU
1	J	164	ALA
1	J	189	ARG
1	J	209	GLU
1	J	211	LEU
1	J	215	VAL
1	J	224	TYR
1	J	228	PRO
1	K	35	THR
1	K	53	VAL
1	K	70	GLY
1	K	78	ILE
1	K	112	GLY
1	K	117	SER
1	K	137	LYS
1	K	138	LEU
1	K	152	PRO
1	K	196	THR

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Mol	Chain	Res	Type
1	K	201	THR
1	K	202	ASP
1	K	204	SER
1	K	208	LEU
2	L	24	GLU
2	L	28	LYS
2	L	43	GLY
2	L	81	ASP
2	L	108	ILE
2	L	112	GLU
2	L	133	ASP
2	L	144	PRO
2	L	157	ARG
2	L	177	GLU
2	L	179	SER
2	L	237	ARG
2	L	316	GLY
2	L	326	ASP
2	L	338	GLU
2	L	381	ALA
2	L	391	LEU
2	L	393	GLN
2	L	423	ALA
2	L	427	VAL
2	L	438	ILE
2	L	445	GLU
2	L	450	GLY
2	L	458	TYR
2	L	460	ARG
2	L	489	SER
2	L	494	TYR
2	L	502	PRO
2	L	508	ILE
2	L	514	VAL
2	L	529	VAL
2	L	534	VAL
2	L	536	PRO
2	L	550	LEU
2	L	560	MET
2	L	582	GLY
2	L	589	ARG
2	L	600	ASP

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Mol	Chain	Res	Type
2	L	605	LYS
2	L	608	GLY
2	L	620	LEU
2	L	635	THR
2	L	655	LEU
2	L	666	LEU
2	L	685	GLU
2	L	698	ASP
2	L	761	PHE
2	L	769	PRO
2	L	775	ARG
2	L	787	ASP
2	L	791	ARG
2	L	793	PRO
2	L	808	ARG
2	L	809	GLY
2	L	855	VAL
2	L	857	ASP
2	L	876	VAL
2	L	877	PRO
2	L	894	GLY
2	L	928	LYS
2	L	933	GLY
2	L	945	ALA
2	L	960	GLU
2	L	968	ASP
2	L	972	VAL
2	L	981	GLU
2	L	987	ILE
2	L	1001	VAL
2	L	1037	VAL
2	L	1046	ALA
2	L	1056	LYS
2	L	1060	ILE
2	L	1066	ALA
2	L	1079	PRO
2	L	1082	PRO
2	L	1083	GLU
2	L	1093	GLN
2	L	1096	ALA
2	L	1106	ASP
2	L	1113	GLU

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Mol	Chain	Res	Type
2	L	1114	GLY
3	M	7	LYS
3	M	14	SER
3	M	18	ILE
3	M	32	ILE
3	M	37	LEU
3	M	43	GLY
3	M	45	PHE
3	M	47	GLU
3	M	67	ARG
3	M	72	VAL
3	M	85	VAL
3	M	99	ALA
3	M	102	ILE
3	M	127	LEU
3	M	129	PHE
3	M	139	GLY
3	M	464	LEU
3	M	480	GLU
3	M	485	SER
3	M	498	VAL
3	M	502	PHE
3	M	506	GLY
3	M	540	LEU
3	M	545	ARG
3	M	558	LEU
3	M	567	ILE
3	M	586	ARG
3	M	595	GLY
3	M	601	ARG
3	M	605	ASP
3	M	609	GLY
3	M	621	LYS
3	M	640	HIS
3	M	643	GLY
3	M	681	ARG
3	M	686	GLU
3	M	689	ASP
3	M	695	ILE
3	M	712	GLY
3	M	715	ALA
3	M	723	GLY

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Mol	Chain	Res	Type
3	M	724	GLN
3	M	735	ALA
3	M	776	GLU
3	M	783	ARG
3	M	784	ASP
3	M	794	GLN
3	M	796	ARG
3	M	803	GLY
3	M	819	GLY
3	M	822	ALA
3	M	864	VAL
3	M	872	ARG
3	M	892	ASP
3	M	893	GLU
3	M	897	GLN
3	M	913	ASP
3	M	920	LEU
3	M	928	ALA
3	M	936	TYR
3	M	958	GLU
3	M	964	LEU
3	M	994	GLN
3	M	1001	GLU
3	M	1020	LEU
3	M	1042	ARG
3	M	1056	PRO
3	M	1070	TYR
3	M	1099	VAL
3	M	1142	SER
3	M	1146	GLY
3	M	1173	PHE
3	M	1175	ILE
3	M	1179	GLU
3	M	1180	ALA
3	M	1188	VAL
3	M	1200	VAL
3	M	1212	ALA
3	M	1215	VAL
3	M	1233	GLY
3	M	1237	THR
3	M	1263	PHE
3	M	1273	VAL

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Mol	Chain	Res	Type
3	M	1287	GLU
3	M	1328	GLY
3	M	1339	LYS
3	M	1353	GLN
3	M	1360	GLY
3	M	1361	VAL
3	M	1365	ASP
3	M	1381	VAL
3	M	1386	ASP
3	M	1397	LYS
3	M	1430	SER
3	M	1449	GLU
3	M	1454	GLY
3	M	1466	VAL
3	M	1473	PRO
3	M	1475	GLY
4	N	6	ILE
4	N	10	PHE
4	N	12	MET
4	N	15	SER
4	N	22	VAL
4	N	23	VAL
4	N	24	ALA
4	N	41	GLU
5	Q	108	LEU
5	Q	111	LEU
5	Q	152	GLY
5	Q	172	GLU
5	Q	173	GLU
5	Q	176	GLY
5	Q	186	LYS
5	Q	277	VAL
5	Q	315	ASP
5	Q	331	SER
5	Q	349	PRO
5	Q	351	GLU
5	Q	387	ARG
5	Q	406	GLY
5	Q	410	GLU
5	Q	419	ALA
5	Q	431	ARG
1	A	7	LYS

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Mol	Chain	Res	Type
1	A	31	GLY
1	A	49	PRO
1	A	74	ASP
1	A	96	SER
1	A	101	LEU
1	A	105	GLY
1	A	109	VAL
1	A	111	ALA
1	A	131	THR
1	A	161	ARG
1	B	32	PHE
1	B	95	ALA
1	B	116	PRO
1	B	132	LEU
1	B	134	GLU
1	B	161	ARG
2	C	14	PRO
2	C	18	LEU
2	C	19	THR
2	C	53	PRO
2	C	166	PRO
2	C	362	GLY
2	C	401	LEU
2	C	410	ILE
2	C	433	THR
2	C	453	THR
2	C	462	ASP
2	C	467	ILE
2	C	486	MET
2	C	507	ARG
2	C	512	ARG
2	C	561	GLY
2	C	575	GLN
2	C	594	ALA
2	C	613	VAL
2	C	625	LEU
2	C	645	VAL
2	C	686	ASP
2	C	696	LYS
2	C	821	GLU
2	C	856	GLU
2	C	873	PRO

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Mol	Chain	Res	Type
2	C	909	ALA
2	C	924	LEU
2	C	936	VAL
2	C	997	LEU
2	C	1020	PRO
2	C	1030	GLN
2	C	1058	ASP
2	C	1069	ALA
2	C	1100	GLN
2	C	1109	VAL
3	D	25	GLU
3	D	44	LEU
3	D	53	ILE
3	D	68	PHE
3	D	133	ILE
3	D	149	LYS
3	D	463	GLU
3	D	561	GLY
3	D	566	ILE
3	D	569	ASN
3	D	579	ASP
3	D	698	LYS
3	D	714	GLN
3	D	818	ARG
3	D	847	ASP
3	D	858	LEU
3	D	904	VAL
3	D	938	GLY
3	D	945	SER
3	D	965	GLU
3	D	967	ALA
3	D	1009	LYS
3	D	1047	LYS
3	D	1048	PRO
3	D	1049	SER
3	D	1098	LEU
3	D	1103	HIS
3	D	1105	ILE
3	D	1128	VAL
3	D	1135	ARG
3	D	1192	LEU
3	D	1315	ASP

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Mol	Chain	Res	Type
3	D	1359	GLN
3	D	1368	ILE
3	D	1387	SER
3	D	1389	LEU
3	D	1416	ALA
3	D	1435	LEU
3	D	1459	LEU
3	D	1465	ASN
3	D	1468	LEU
3	D	1485	GLN
4	E	18	ARG
4	E	71	GLY
4	E	84	ARG
5	H	181	LEU
5	H	297	LEU
5	H	327	GLN
5	H	353	LEU
1	J	7	LYS
1	J	31	GLY
1	J	49	PRO
1	J	74	ASP
1	J	96	SER
1	J	101	LEU
1	J	105	GLY
1	J	109	VAL
1	J	111	ALA
1	J	131	THR
1	J	161	ARG
1	K	32	PHE
1	K	95	ALA
1	K	116	PRO
1	K	132	LEU
1	K	134	GLU
1	K	161	ARG
2	L	14	PRO
2	L	18	LEU
2	L	19	THR
2	L	53	PRO
2	L	166	PRO
2	L	362	GLY
2	L	401	LEU
2	L	410	ILE

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Mol	Chain	Res	Type
2	L	433	THR
2	L	453	THR
2	L	462	ASP
2	L	467	ILE
2	L	486	MET
2	L	507	ARG
2	L	512	ARG
2	L	561	GLY
2	L	575	GLN
2	L	594	ALA
2	L	613	VAL
2	L	625	LEU
2	L	645	VAL
2	L	686	ASP
2	L	696	LYS
2	L	821	GLU
2	L	856	GLU
2	L	873	PRO
2	L	909	ALA
2	L	924	LEU
2	L	936	VAL
2	L	997	LEU
2	L	1020	PRO
2	L	1030	GLN
2	L	1058	ASP
2	L	1069	ALA
2	L	1100	GLN
2	L	1109	VAL
3	M	25	GLU
3	M	44	LEU
3	M	53	ILE
3	M	68	PHE
3	M	133	ILE
3	M	149	LYS
3	M	463	GLU
3	M	561	GLY
3	M	566	ILE
3	M	569	ASN
3	M	579	ASP
3	M	698	LYS
3	M	714	GLN
3	M	818	ARG

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Mol	Chain	Res	Type
3	M	847	ASP
3	M	858	LEU
3	M	883	ALA
3	M	904	VAL
3	M	938	GLY
3	M	945	SER
3	M	965	GLU
3	M	967	ALA
3	M	1009	LYS
3	M	1047	LYS
3	M	1048	PRO
3	M	1049	SER
3	M	1098	LEU
3	M	1103	HIS
3	M	1105	ILE
3	M	1128	VAL
3	M	1135	ARG
3	M	1192	LEU
3	M	1315	ASP
3	M	1359	GLN
3	M	1368	ILE
3	M	1387	SER
3	M	1389	LEU
3	M	1416	ALA
3	M	1435	LEU
3	M	1459	LEU
3	M	1465	ASN
3	M	1468	LEU
3	M	1485	GLN
4	N	18	ARG
4	N	71	GLY
4	N	84	ARG
5	Q	181	LEU
5	Q	297	LEU
5	Q	327	GLN
5	Q	353	LEU
1	A	78	ILE
1	A	91	ASP
1	A	128	HIS
1	A	152	PRO
1	A	218	LEU
1	B	13	ALA

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Mol	Chain	Res	Type
1	B	20	TYR
1	B	21	GLY
1	B	22	GLU
1	B	46	SER
1	B	48	ILE
1	B	76	VAL
1	B	113	ASP
2	C	35	PRO
2	C	87	ASP
2	C	106	GLY
2	C	148	PHE
2	C	167	LYS
2	C	175	GLU
2	C	205	GLU
2	C	303	PHE
2	C	317	VAL
2	C	318	PRO
2	C	376	ARG
2	C	394	PHE
2	C	521	PRO
2	C	562	SER
2	C	572	ILE
2	C	607	ASP
2	C	636	ALA
2	C	659	PRO
2	C	675	ALA
2	C	682	TYR
2	C	716	LYS
2	C	739	GLU
2	C	756	VAL
2	C	777	ILE
2	C	786	LYS
2	C	796	GLU
2	C	822	VAL
2	C	830	LYS
2	C	833	LEU
2	C	834	GLN
2	C	942	GLU
2	C	943	VAL
2	C	1039	ALA
2	C	1072	LYS
2	C	1089	VAL

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Mol	Chain	Res	Type
3	D	6	ARG
3	D	101	HIS
3	D	135	LEU
3	D	136	ASP
3	D	457	GLY
3	D	468	LEU
3	D	490	ALA
3	D	496	LEU
3	D	520	LEU
3	D	546	ARG
3	D	554	LEU
3	D	570	GLU
3	D	592	THR
3	D	594	PRO
3	D	608	SER
3	D	644	LEU
3	D	666	PHE
3	D	673	ALA
3	D	721	VAL
3	D	765	SER
3	D	785	ILE
3	D	843	PHE
3	D	883	ALA
3	D	934	LEU
3	D	944	THR
3	D	976	GLN
3	D	1069	GLU
3	D	1101	VAL
3	D	1115	THR
3	D	1177	ALA
3	D	1193	THR
3	D	1274	ILE
3	D	1277	ILE
3	D	1342	GLU
3	D	1352	ILE
3	D	1354	LYS
3	D	1377	LYS
3	D	1432	LYS
3	D	1460	ILE
4	E	26	ARG
4	E	73	LEU
4	E	79	LEU

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Mol	Chain	Res	Type
5	H	110	THR
5	H	217	TYR
5	H	222	LEU
5	H	271	ARG
5	H	310	MET
5	H	323	LEU
5	H	354	PRO
5	H	393	GLY
5	H	403	ALA
1	J	78	ILE
1	J	91	ASP
1	J	128	HIS
1	J	152	PRO
1	J	218	LEU
1	K	13	ALA
1	K	20	TYR
1	K	21	GLY
1	K	22	GLU
1	K	46	SER
1	K	48	ILE
1	K	76	VAL
1	K	113	ASP
2	L	35	PRO
2	L	87	ASP
2	L	106	GLY
2	L	148	PHE
2	L	167	LYS
2	L	175	GLU
2	L	205	GLU
2	L	303	PHE
2	L	317	VAL
2	L	318	PRO
2	L	376	ARG
2	L	394	PHE
2	L	521	PRO
2	L	562	SER
2	L	572	ILE
2	L	607	ASP
2	L	636	ALA
2	L	659	PRO
2	L	675	ALA
2	L	682	TYR

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Mol	Chain	Res	Type
2	L	716	LYS
2	L	739	GLU
2	L	756	VAL
2	L	777	ILE
2	L	786	LYS
2	L	796	GLU
2	L	822	VAL
2	L	830	LYS
2	L	833	LEU
2	L	834	GLN
2	L	942	GLU
2	L	943	VAL
2	L	1039	ALA
2	L	1072	LYS
2	L	1089	VAL
3	M	6	ARG
3	M	101	HIS
3	M	135	LEU
3	M	136	ASP
3	M	457	GLY
3	M	468	LEU
3	M	490	ALA
3	M	496	LEU
3	M	520	LEU
3	M	546	ARG
3	M	554	LEU
3	M	570	GLU
3	M	592	THR
3	M	594	PRO
3	M	608	SER
3	M	644	LEU
3	M	666	PHE
3	M	673	ALA
3	M	721	VAL
3	M	765	SER
3	M	785	ILE
3	M	843	PHE
3	M	934	LEU
3	M	944	THR
3	M	976	GLN
3	M	1069	GLU
3	M	1101	VAL

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Mol	Chain	Res	Type
3	M	1115	THR
3	M	1177	ALA
3	M	1193	THR
3	M	1274	ILE
3	M	1277	ILE
3	M	1342	GLU
3	M	1352	ILE
3	M	1354	LYS
3	M	1377	LYS
3	M	1432	LYS
3	M	1460	ILE
4	N	26	ARG
4	N	73	LEU
4	N	79	LEU
5	Q	110	THR
5	Q	217	TYR
5	Q	222	LEU
5	Q	271	ARG
5	Q	310	MET
5	Q	323	LEU
5	Q	354	PRO
5	Q	393	GLY
5	Q	403	ALA
1	A	41	ARG
1	A	45	LEU
1	A	53	VAL
1	A	127	LEU
1	A	139	TYR
1	A	203	GLY
1	B	119	ASP
1	B	154	GLU
1	B	175	ARG
1	B	187	GLY
2	C	15	LEU
2	C	21	ILE
2	C	73	ILE
2	C	124	ASP
2	C	149	THR
2	C	231	PRO
2	C	235	MET
2	C	243	ARG
2	C	377	PRO

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Mol	Chain	Res	Type
2	C	407	LYS
2	C	576	ALA
2	C	624	PRO
2	C	681	GLY
2	C	889	HIS
2	C	925	TYR
2	C	958	SER
2	C	966	LEU
2	C	977	GLY
2	C	1047	HIS
2	C	1063	ARG
2	C	1101	THR
3	D	150	ARG
3	D	743	ASP
3	D	774	SER
3	D	816	TYR
3	D	906	GLN
3	D	929	ARG
3	D	972	ARG
3	D	1012	GLU
3	D	1107	VAL
3	D	1133	ARG
3	D	1136	LYS
3	D	1207	TYR
3	D	1229	ILE
3	D	1299	PHE
3	D	1317	ASP
3	D	1324	PRO
4	E	55	TYR
5	H	138	ASP
5	H	154	ALA
5	H	355	SER
1	J	41	ARG
1	J	45	LEU
1	J	53	VAL
1	J	127	LEU
1	J	139	TYR
1	J	203	GLY
1	K	119	ASP
1	K	154	GLU
1	K	175	ARG
1	K	187	GLY

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Mol	Chain	Res	Type
2	L	15	LEU
2	L	21	ILE
2	L	73	ILE
2	L	124	ASP
2	L	149	THR
2	L	231	PRO
2	L	235	MET
2	L	243	ARG
2	L	377	PRO
2	L	407	LYS
2	L	576	ALA
2	L	624	PRO
2	L	681	GLY
2	L	889	HIS
2	L	925	TYR
2	L	958	SER
2	L	966	LEU
2	L	977	GLY
2	L	1047	HIS
2	L	1063	ARG
2	L	1101	THR
3	M	150	ARG
3	M	743	ASP
3	M	774	SER
3	M	816	TYR
3	M	906	GLN
3	M	929	ARG
3	M	972	ARG
3	M	1012	GLU
3	M	1107	VAL
3	M	1133	ARG
3	M	1136	LYS
3	M	1207	TYR
3	M	1229	ILE
3	M	1299	PHE
3	M	1317	ASP
3	M	1324	PRO
4	N	55	TYR
5	Q	138	ASP
5	Q	154	ALA
5	Q	355	SER
1	A	58	ILE

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Mol	Chain	Res	Type
1	A	75	VAL
2	C	9	ILE
2	C	23	VAL
2	C	197	LEU
2	C	390	GLN
2	C	403	SER
2	C	602	GLU
2	C	794	PRO
2	C	835	VAL
2	C	858	MET
2	C	859	PRO
3	D	504	ASP
3	D	623	VAL
3	D	882	PHE
3	D	884	ARG
3	D	981	GLY
3	D	987	GLU
3	D	989	TYR
3	D	1007	VAL
3	D	1213	ARG
3	D	1290	LEU
3	D	1319	VAL
3	D	1443	THR
3	D	1478	SER
5	H	244	TYR
5	H	302	SER
1	J	58	ILE
1	J	75	VAL
2	L	9	ILE
2	L	23	VAL
2	L	197	LEU
2	L	390	GLN
2	L	403	SER
2	L	500	ASN
2	L	602	GLU
2	L	794	PRO
2	L	835	VAL
2	L	858	MET
2	L	859	PRO
2	L	947	ALA
3	M	504	ASP
3	M	623	VAL

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Mol	Chain	Res	Type
3	M	882	PHE
3	M	884	ARG
3	M	981	GLY
3	M	987	GLU
3	M	1007	VAL
3	M	1213	ARG
3	M	1290	LEU
3	M	1319	VAL
3	M	1443	THR
3	M	1478	SER
5	Q	244	TYR
5	Q	302	SER
2	C	181	VAL
2	C	287	GLY
2	C	304	LEU
2	C	443	THR
2	C	520	GLU
2	C	912	PRO
2	C	1033	GLY
3	D	108	VAL
3	D	144	GLY
3	D	1032	PRO
3	D	1221	VAL
3	D	1392	GLY
2	L	181	VAL
2	L	287	GLY
2	L	304	LEU
2	L	443	THR
2	L	520	GLU
2	L	912	PRO
2	L	1033	GLY
3	M	108	VAL
3	M	144	GLY
3	M	1032	PRO
3	M	1221	VAL
3	M	1392	GLY
1	A	21	GLY
1	A	92	PRO
1	B	129	ILE
1	B	199	ILE
2	C	119	PRO
2	C	192	PRO

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Mol	Chain	Res	Type
2	C	446	GLY
2	C	678	PRO
2	C	727	PRO
3	D	719	VAL
3	D	792	ILE
3	D	992	VAL
3	D	1372	VAL
3	D	1415	VAL
3	D	1461	GLY
5	H	210	VAL
5	H	356	PRO
1	J	21	GLY
1	J	92	PRO
1	K	129	ILE
1	K	199	ILE
2	L	119	PRO
2	L	192	PRO
2	L	446	GLY
2	L	678	PRO
2	L	727	PRO
3	M	719	VAL
3	M	761	ILE
3	M	792	ILE
3	M	992	VAL
3	M	1372	VAL
3	M	1415	VAL
3	M	1461	GLY
5	Q	210	VAL
5	Q	356	PRO
1	B	124	ASN
2	C	151	ASP
2	C	319	GLY
2	C	415	PRO
2	C	621	VAL
2	C	674	VAL
2	C	799	ILE
2	C	982	PRO
2	C	1077	PRO
2	C	1099	VAL
3	D	683	ILE
3	D	761	ILE
3	D	809	PRO

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Mol	Chain	Res	Type
3	D	856	GLY
1	K	124	ASN
2	L	151	ASP
2	L	319	GLY
2	L	415	PRO
2	L	621	VAL
2	L	674	VAL
2	L	799	ILE
2	L	982	PRO
2	L	1077	PRO
2	L	1099	VAL
3	M	683	ILE
3	M	809	PRO
3	M	856	GLY
2	C	852	ILE
2	C	1055	ILE
3	D	38	LYS
2	L	852	ILE
2	L	1055	ILE
3	M	38	LYS
2	C	757	GLY
2	C	1016	ILE
2	C	1076	VAL
3	D	137	PRO
3	D	599	PRO
3	D	632	VAL
3	D	974	ILE
3	D	1423	GLY
3	D	1467	ILE
2	L	757	GLY
2	L	1016	ILE
2	L	1076	VAL
3	M	137	PRO
3	M	632	VAL
3	M	974	ILE
3	M	1423	GLY
3	M	1467	ILE

### 5.3.2 Protein sidechains ⓘ

There are no protein residues with a non-rotameric sidechain to report in this entry.



### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	D	11
3	M	11
2	C	8
2	L	8
5	Q	1
5	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	44:LEU	C	45:PHE	N	1.70
1	M	44:LEU	C	45:PHE	N	1.70
1	D	532:GLY	C	533:GLY	N	1.61
1	M	532:GLY	C	533:GLY	N	1.61
1	C	416:GLY	C	417:GLY	N	1.19
1	L	416:GLY	C	417:GLY	N	1.19
1	D	93:ILE	C	94:GLU	N	1.17
1	M	93:ILE	C	94:GLU	N	1.17
1	D	115:LEU	C	116:LEU	N	1.16
1	M	115:LEU	C	116:LEU	N	1.16
1	C	423:ALA	C	424:GLY	N	1.13
1	L	423:ALA	C	424:GLY	N	1.13
1	D	113:GLY	C	114:THR	N	1.12
1	M	113:GLY	C	114:THR	N	1.12
1	D	1087:ARG	C	1088:THR	N	1.11
1	M	1087:ARG	C	1088:THR	N	1.11
1	D	521:PRO	C	522:PRO	N	1.09
1	D	526:PRO	C	527:MET	N	1.09
1	M	521:PRO	C	522:PRO	N	1.09
1	M	526:PRO	C	527:MET	N	1.09
1	D	529:GLN	C	530:VAL	N	1.06
1	M	529:GLN	C	530:VAL	N	1.06
1	H	239:VAL	C	240:GLU	N	1.05
1	Q	239:VAL	C	240:GLU	N	1.05
1	C	418:LEU	C	419:THR	N	1.01
1	C	419:THR	C	420:ARG	N	1.01
1	C	422:ARG	C	423:ALA	N	1.01
1	L	418:LEU	C	419:THR	N	1.01
1	L	419:THR	C	420:ARG	N	1.01
1	L	422:ARG	C	423:ALA	N	1.01
1	D	531:ASP	C	532:GLY	N	1.00
1	M	531:ASP	C	532:GLY	N	1.00
1	C	240:THR	C	241:LEU	N	0.99
1	L	240:THR	C	241:LEU	N	0.98
1	C	417:GLY	C	418:LEU	N	0.95
1	L	417:GLY	C	418:LEU	N	0.95
1	C	244:PRO	C	245:GLY	N	0.92
1	D	91:GLY	C	92:HIS	N	0.92
1	L	244:PRO	C	245:GLY	N	0.92
1	M	91:GLY	C	92:HIS	N	0.92

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.