



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 06:37 am GMT

PDB ID : 1PQV  
Title : RNA polymerase II-TFIIS complex  
Authors : Kettenberger, H.; Armache, K.-J.; Cramer, P.  
Deposited on : 2003-06-19  
Resolution : 3.80 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

<http://wwpdb.org/validation/2016/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)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

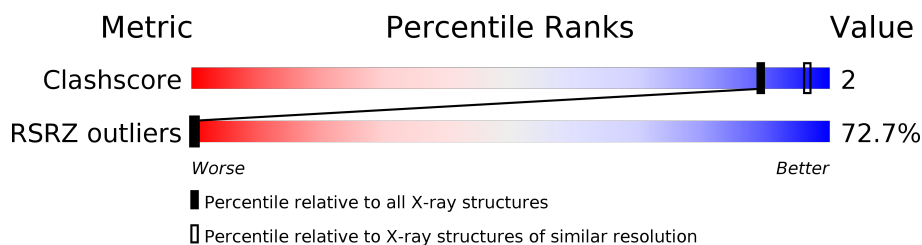
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

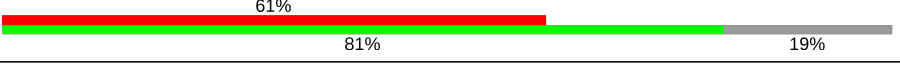
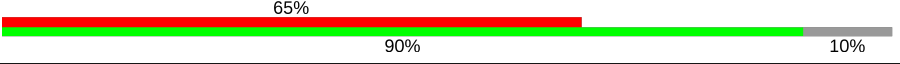

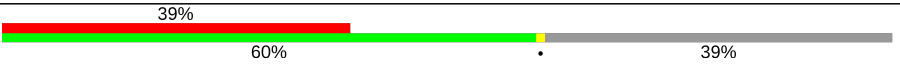
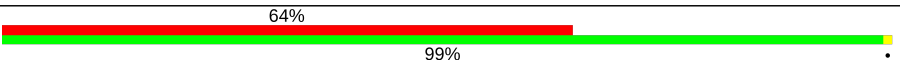

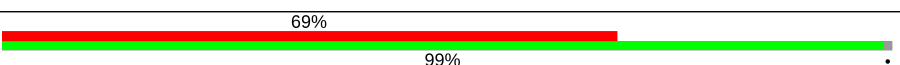
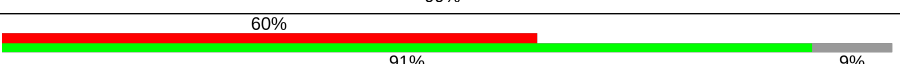
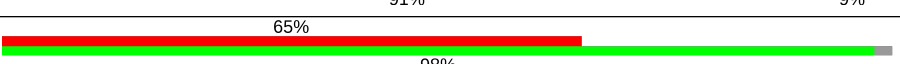
The reported resolution of this entry is 3.80 Å.

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	112137	1030 (4.04-3.56)
RSRZ outliers	101464	1032 (4.08-3.52)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1733	
2	B	1224	
3	C	318	
4	D	221	
5	E	215	
6	F	155	
7	G	171	
8	H	146	
9	I	122	

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Mol	Chain	Length	Quality of chain
10	J	70	<div><div></div><div>73%93%7%</div></div>
11	K	120	<div><div></div><div>76%95%5%</div></div>
12	L	70	<div><div></div><div>41%66%34%</div></div>
13	S	309	<div><div></div><div>40%54%.44%</div></div>

## 2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 4041 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 II largest subunit.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
1	A	1409	Total	C	0	0	1409
			1409	1409			

- Molecule 2 is a protein called DNA-directed RNA polymerase II 140 kDa polypeptide.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
2	B	1103	Total	C	0	0	1103
			1103	1103			

- Molecule 3 is a protein called DNA-directed RNA polymerase II 45 kDa polypeptide.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
3	C	266	Total	C	0	0	266
			266	266			

- Molecule 4 is a protein called DNA-directed RNA polymerase II 32 kDa polypeptide.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
4	D	135	Total	C	0	0	135
			135	135			

There are 29 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	86	UNK	-	SEE REMARK 999	UNP P20433
D	87	UNK	-	SEE REMARK 999	UNP P20433
D	88	UNK	-	SEE REMARK 999	UNP P20433
D	89	UNK	-	SEE REMARK 999	UNP P20433
D	90	UNK	-	SEE REMARK 999	UNP P20433
D	91	UNK	-	SEE REMARK 999	UNP P20433
D	92	UNK	-	SEE REMARK 999	UNP P20433
D	93	UNK	-	SEE REMARK 999	UNP P20433

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Chain	Residue	Modelled	Actual	Comment	Reference
D	94	UNK	-	SEE REMARK 999	UNP P20433
D	95	UNK	-	SEE REMARK 999	UNP P20433
D	96	UNK	-	SEE REMARK 999	UNP P20433
D	97	UNK	-	SEE REMARK 999	UNP P20433
D	98	UNK	-	SEE REMARK 999	UNP P20433
D	99	UNK	-	SEE REMARK 999	UNP P20433
D	100	UNK	-	SEE REMARK 999	UNP P20433
D	101	UNK	-	SEE REMARK 999	UNP P20433
D	102	UNK	-	SEE REMARK 999	UNP P20433
D	103	UNK	-	SEE REMARK 999	UNP P20433
D	104	UNK	-	SEE REMARK 999	UNP P20433
D	105	UNK	-	SEE REMARK 999	UNP P20433
D	106	UNK	-	SEE REMARK 999	UNP P20433
D	107	UNK	-	SEE REMARK 999	UNP P20433
D	108	UNK	-	SEE REMARK 999	UNP P20433
D	109	UNK	-	SEE REMARK 999	UNP P20433
D	110	UNK	-	SEE REMARK 999	UNP P20433
D	111	UNK	-	SEE REMARK 999	UNP P20433
D	112	UNK	-	SEE REMARK 999	UNP P20433
D	113	UNK	-	SEE REMARK 999	UNP P20433
D	114	UNK	-	SEE REMARK 999	UNP P20433

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	E	214	Total C 214 214	0	0	214

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	F	84	Total C 84 84	0	0	84

- Molecule 7 is a protein called DNA-directed RNA polymerase II 19 kDa polypeptide.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
7	G	169	Total C 169 169	0	0	169

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
8	H	133	Total	C	0	0	133
			133	133			

- Molecule 9 is a protein called DNA-directed RNA polymerase II 14.2 kDa polypeptide.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
9	I	119	Total	C	0	0	119
			119	119			

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III 8.3 kDa polypeptide.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
10	J	65	Total	C	0	0	65
			65	65			

- Molecule 11 is a protein called DNA-directed RNA polymerase II 13.6 kDa polypeptide.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
11	K	114	Total	C	0	0	114
			114	114			

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
12	L	46	Total	C	0	0	46
			46	46			

- Molecule 13 is a protein called Transcription elongation factor S-II.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
13	S	174	Total	C	0	0	174
			174	174			

- Molecule 14 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	1	Total	Mg	0	0
			1	1		

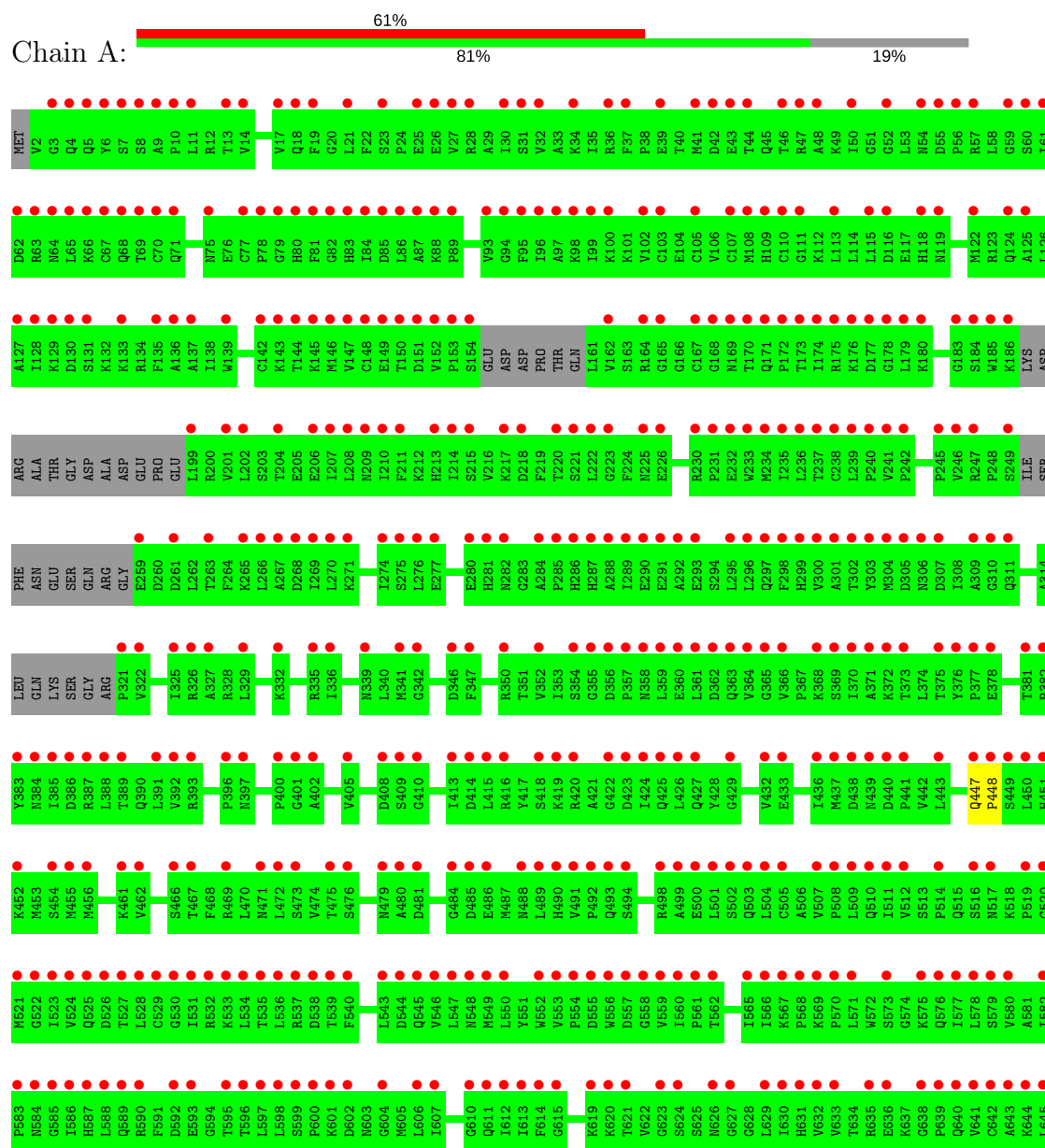
- Molecule 15 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	J	1	Total 1	Zn 1	0	0
15	B	1	Total 1	Zn 1	0	0
15	I	2	Total 2	Zn 2	0	0
15	C	1	Total 1	Zn 1	0	0
15	A	2	Total 2	Zn 2	0	0
15	L	1	Total 1	Zn 1	0	0
15	S	1	Total 1	Zn 1	0	0

### 3 Residue-property plots

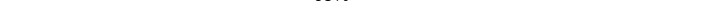
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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 II largest subunit





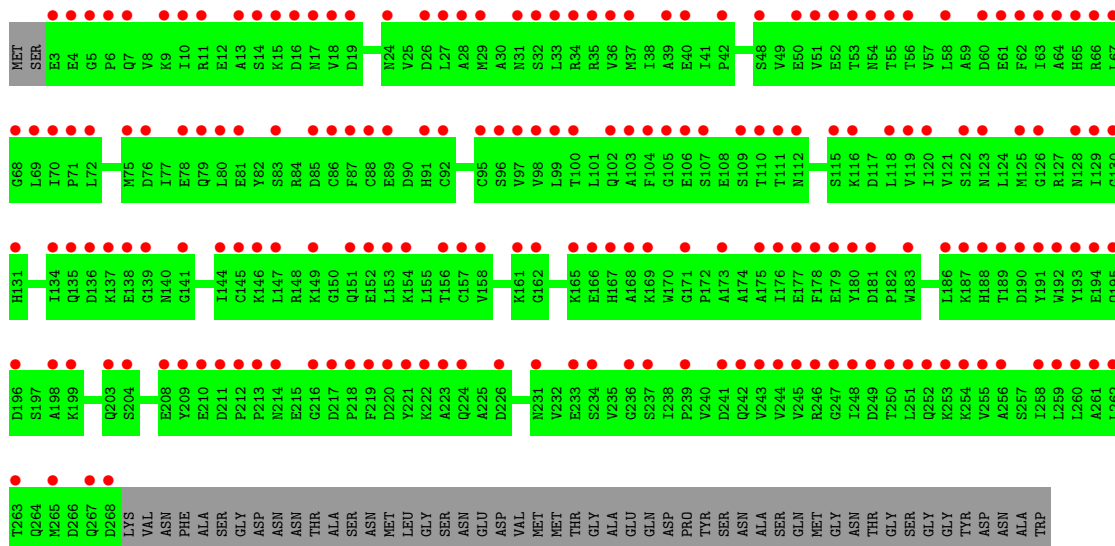
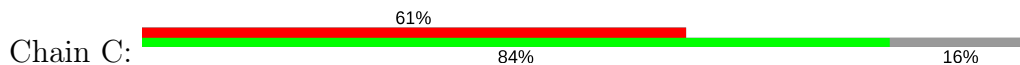


Chain B:  65% 90% 10%

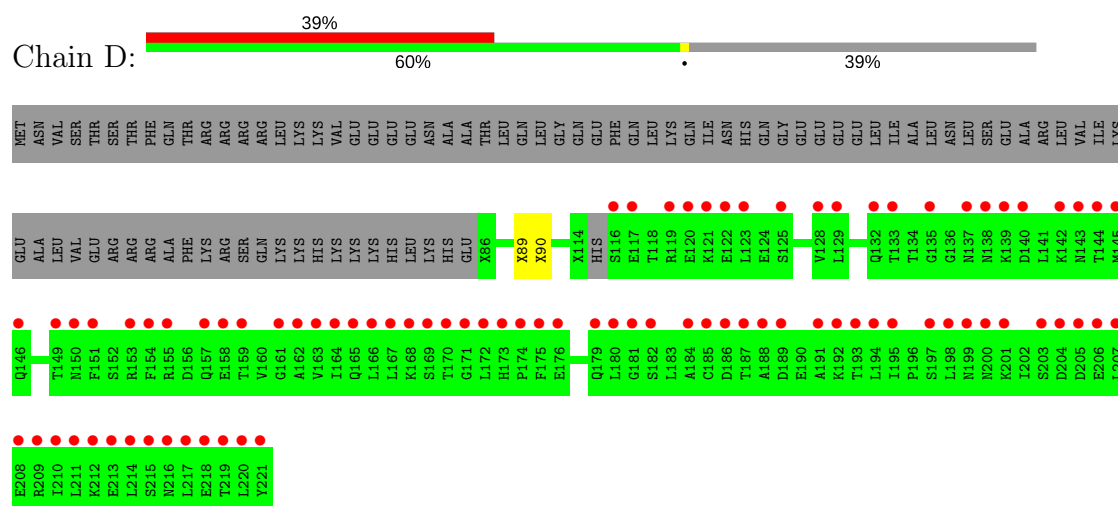




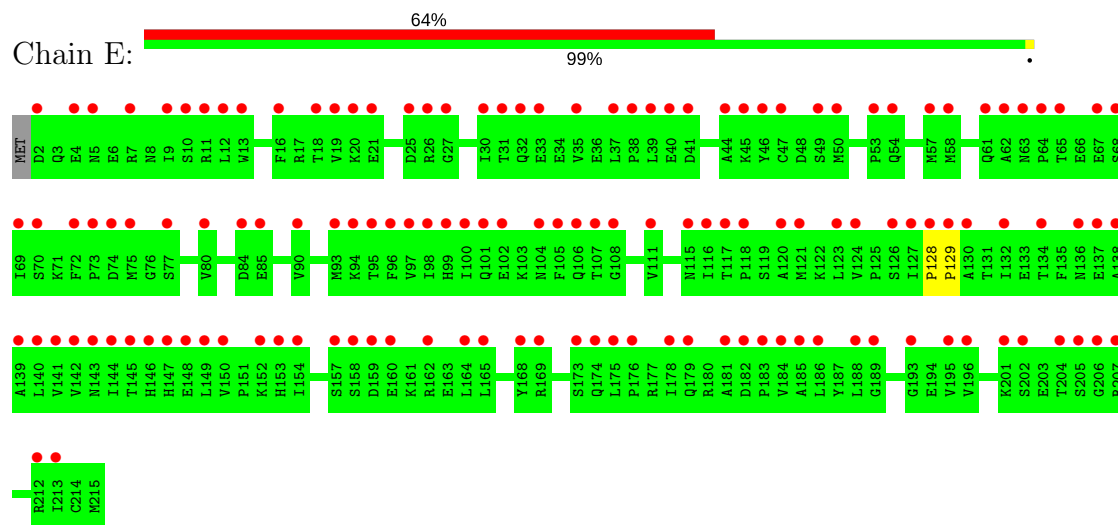
• Molecule 3: DNA-directed RNA polymerase II 45 kDa polypeptide



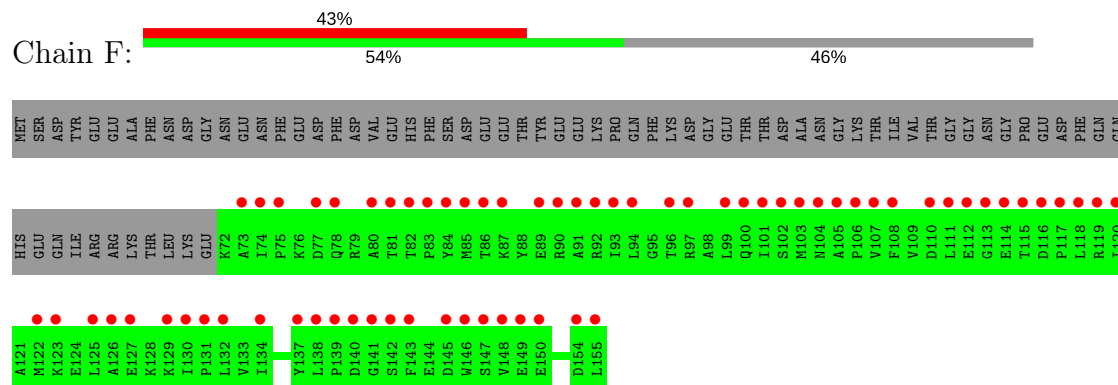
• Molecule 4: DNA-directed RNA polymerase II 32 kDa polypeptide



- Molecule 5: DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide

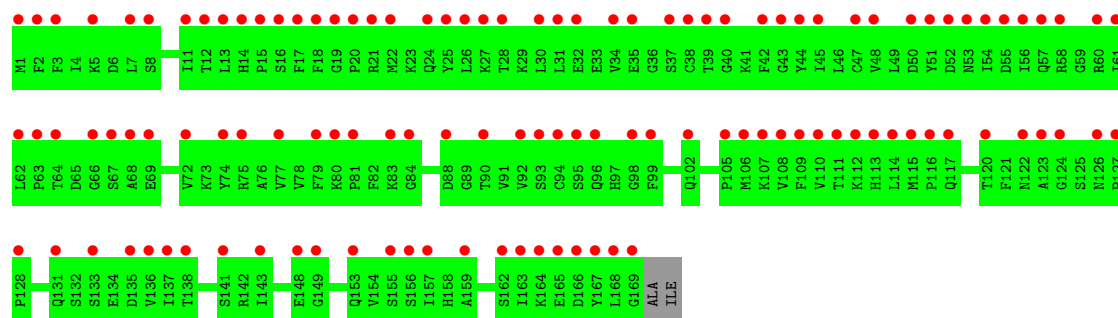


- Molecule 6: DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide

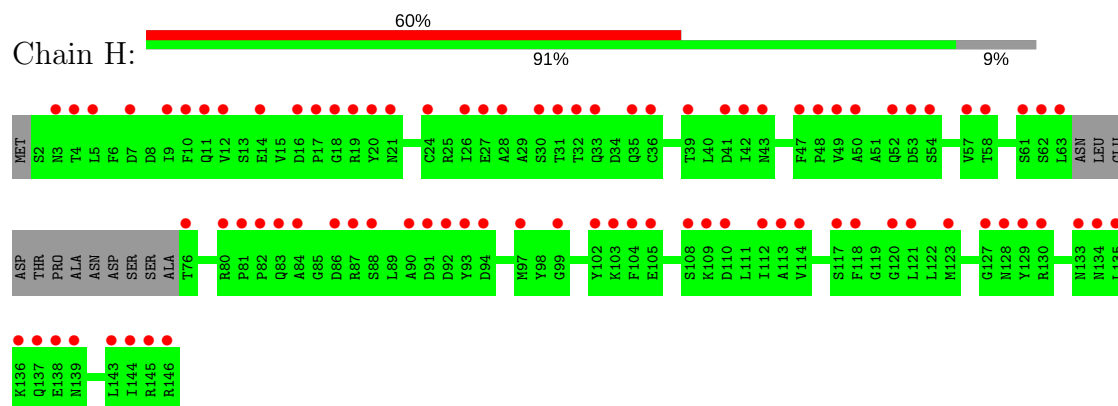


- Molecule 7: DNA-directed RNA polymerase II 19 kDa polypeptide

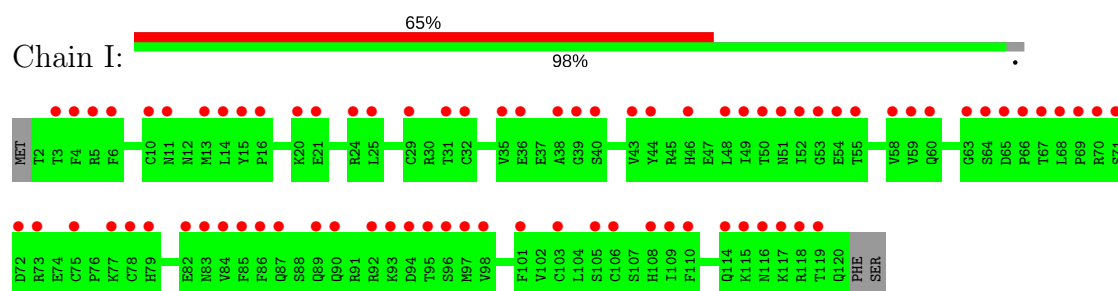




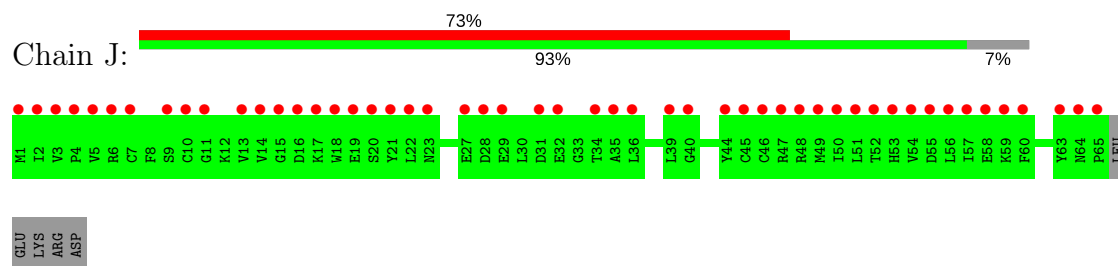
- Molecule 8: DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide



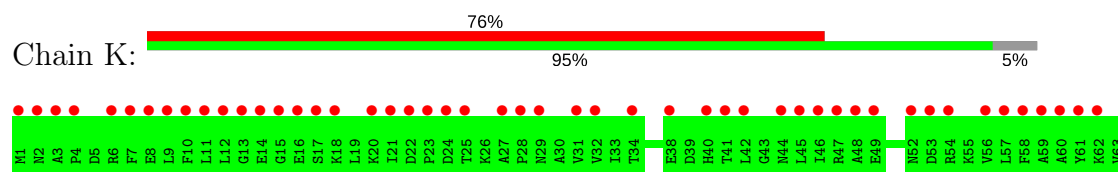
- Molecule 9: DNA-directed RNA polymerase II 14.2 kDa polypeptide



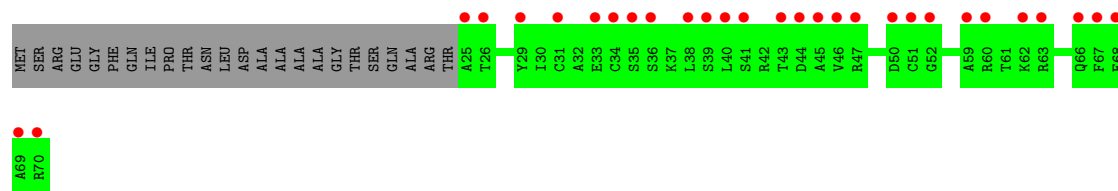
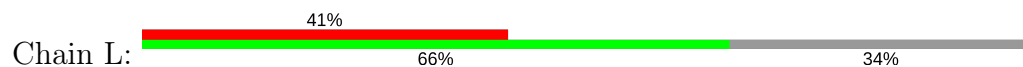
- Molecule 10: DNA-directed RNA polymerases I, II, and III 8.3 kDa polypeptide



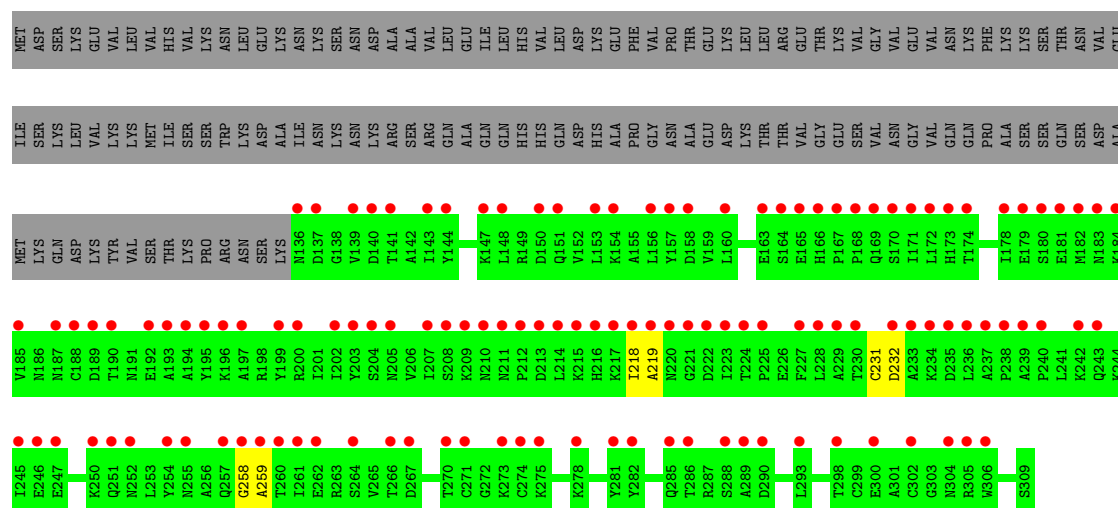
- Molecule 11: DNA-directed RNA polymerase II 13.6 kDa polypeptide



- Molecule 12: DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide



- Molecule 13: Transcription elongation factor S-II



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	218.90Å 395.30Å 281.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.80 49.41 – 3.79	Depositor EDS
% Data completeness (in resolution range)	96.2 (50.00-3.80) 89.4 (49.41-3.79)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.66 (at 3.77Å)	Xtriage
Refinement program	O	Depositor
R, $R_{free}$	(Not available) , (Not available) 0.464 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	93.6	Xtriage
Anisotropy	0.465	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 91.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.013 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.022 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
$F_o, F_c$ correlation	0.62	EDS
Total number of atoms	4041	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.17% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1409	0	0	3	0
2	B	1103	0	0	1	0
3	C	266	0	0	0	0
4	D	135	0	0	1	0
5	E	214	0	0	1	0
6	F	84	0	0	0	0
7	G	169	0	0	0	0
8	H	133	0	0	0	0
9	I	119	0	0	0	0
10	J	65	0	0	0	0
11	K	114	0	0	0	0
12	L	46	0	0	0	0
13	S	174	0	0	3	0
14	A	1	0	0	0	0
15	A	2	0	0	0	0
15	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	C	1	0	0	0	0
15	I	2	0	0	0	0
15	J	1	0	0	0	0
15	L	1	0	0	0	0
15	S	1	0	0	0	0
All	All	4041	0	0	9	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 2.

All (9) 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)
1:A:1330:ASN:CA	1:A:1331:SER:CA	2.54	0.85
4:D:89:UNK:CA	4:D:90:UNK:CA	2.57	0.83
1:A:1385:THR:CA	1:A:1386:ARG:CA	2.57	0.81
2:B:505:ASP:CA	2:B:506:GLY:CA	2.63	0.76
13:S:218:ILE:CA	13:S:219:ALA:CA	2.73	0.66
13:S:231:CYS:CA	13:S:232:ASP:CA	2.86	0.53
5:E:128:PRO:CA	5:E:129:PRO:CA	2.91	0.49
1:A:447:GLN:CA	1:A:448:PRO:CA	2.90	0.49
13:S:258:GLY:CA	13:S:259:ALA:CA	2.99	0.41

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

### 5.3.2 Protein sidechains [i](#)

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 10 ligands modelled in this entry, 10 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1409/1733 (81%)	4.65	1053 (74%)  	30, 30, 30, 30	0
2	B	1103/1224 (90%)	4.81	791 (71%)  	30, 30, 30, 30	0
3	C	266/318 (83%)	4.63	194 (72%)  	30, 30, 30, 30	0
4	D	106/221 (47%)	6.18	86 (81%)  	30, 30, 30, 30	0
5	E	214/215 (99%)	4.31	138 (64%)  	30, 30, 30, 30	0
6	F	84/155 (54%)	5.41	67 (79%)  	30, 30, 30, 30	0
7	G	169/171 (98%)	5.60	118 (69%)  	30, 30, 30, 30	0
8	H	133/146 (91%)	4.99	87 (65%)  	30, 30, 30, 30	0
9	I	119/122 (97%)	5.60	79 (66%)  	30, 30, 30, 30	0
10	J	65/70 (92%)	5.71	51 (78%)  	30, 30, 30, 30	0
11	K	114/120 (95%)	5.25	91 (79%)  	30, 30, 30, 30	0
12	L	46/70 (65%)	5.02	29 (63%)  	30, 30, 30, 30	0
13	S	174/309 (56%)	4.96	124 (71%)  	30, 30, 30, 30	0
All	All	4002/4874 (82%)	4.86	2908 (72%)  	30, 30, 30, 30	0

All (2908) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	306	ASN	44.9
2	B	275	TYR	40.4
7	G	113	HIS	37.9
9	I	3	THR	34.5
1	A	1272	THR	33.5
12	L	26	THR	31.7
2	B	735	ALA	30.8
2	B	69	LEU	30.2
2	B	274	PRO	29.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
9	I	51	ASN	28.1
5	E	138	ALA	27.6
2	B	568	ASP	27.4
10	J	65	PRO	27.1
1	A	1083	THR	26.6
1	A	423	ASP	26.5
8	H	90	ALA	25.0
2	B	515	HIS	24.4
1	A	420	ARG	24.3
9	I	72	ASP	24.2
2	B	295	GLY	23.6
2	B	781	PHE	23.1
8	H	121	LEU	23.0
2	B	212	LEU	22.9
1	A	1320	PRO	22.0
2	B	1108	ARG	21.9
5	E	115	ASN	21.9
3	C	109	SER	21.8
13	S	189	ASP	21.8
1	A	555	ASP	21.8
8	H	48	PRO	21.8
1	A	214	ILE	21.7
8	H	87	ARG	21.5
9	I	58	VAL	21.5
9	I	97	MET	21.5
1	A	560	ILE	21.4
4	D	158	GLU	21.2
3	C	56	THR	21.1
11	K	84	LYS	20.8
6	F	115	THR	20.8
1	A	537	ARG	20.7
7	G	165	GLU	20.4
13	S	237	ALA	20.4
13	S	290	ASP	20.4
2	B	279	ASP	20.3
1	A	702	LEU	20.2
13	S	137	ASP	20.1
2	B	293	PRO	20.1
1	A	64	ASN	20.1
1	A	1186	ASP	20.0
1	A	955	PRO	19.9
9	I	96	SER	19.9

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Mol	Chain	Res	Type	RSRZ
2	B	860	MET	19.9
7	G	18	PHE	19.9
3	C	211	ASP	19.8
13	S	143	ILE	19.8
4	D	137	ASN	19.7
1	A	1129	GLU	19.7
2	B	886	LYS	19.4
2	B	1190	ASP	19.4
7	G	28	THR	19.3
2	B	320	ASP	19.3
9	I	52	ILE	19.1
10	J	64	ASN	19.0
1	A	170	THR	18.9
2	B	597	MET	18.9
1	A	115	LEU	18.7
3	C	217	ASP	18.7
1	A	437	MET	18.4
2	B	1211	ASN	18.3
4	D	207	LEU	18.1
3	C	224	GLN	18.1
1	A	171	GLN	18.1
4	D	180	LEU	18.1
7	G	96	GLN	18.0
2	B	200	GLY	18.0
7	G	31	LEU	18.0
4	D	201	LYS	17.9
8	H	31	THR	17.7
1	A	108	MET	17.6
1	A	582	ILE	17.5
2	B	509	ALA	17.5
4	D	214	LEU	17.5
8	H	4	THR	17.5
2	B	334	ILE	17.5
4	D	211	LEU	17.4
2	B	171	PRO	17.4
1	A	1112	LYS	17.4
1	A	88	LYS	17.4
11	K	25	THR	17.4
2	B	786	ASN	17.3
1	A	1257	ASP	17.2
4	D	210	ILE	17.2
7	G	135	ASP	17.1

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Mol	Chain	Res	Type	RSRZ
7	G	63	PRO	17.0
3	C	194	GLU	16.7
13	S	172	LEU	16.7
13	S	222	ASP	16.7
5	E	73	PRO	16.6
1	A	568	PRO	16.5
1	A	996	ASN	16.3
3	C	26	ASP	16.3
8	H	80	ARG	16.3
1	A	215	SER	16.2
6	F	107	VAL	16.2
11	K	52	ASN	16.2
1	A	103	CYS	16.1
8	H	129	TYR	15.9
9	I	78	CYS	15.9
2	B	501	PRO	15.9
8	H	35	GLN	15.8
12	L	41	SER	15.8
4	D	172	LEU	15.8
2	B	816	GLU	15.8
2	B	711	GLU	15.7
7	G	120	THR	15.7
1	A	1158	PRO	15.7
2	B	661	LEU	15.7
8	H	53	ASP	15.7
11	K	68	PHE	15.6
2	B	554	ILE	15.5
13	S	166	HIS	15.5
2	B	1048	THR	15.5
2	B	836	GLU	15.5
2	B	525	ALA	15.5
1	A	1254	ALA	15.5
2	B	866	TYR	15.5
2	B	533	CYS	15.4
2	B	354	ASP	15.4
2	B	313	MET	15.4
2	B	546	SER	15.4
1	A	36	ARG	15.4
7	G	88	ASP	15.3
1	A	597	LEU	15.2
2	B	432	MET	15.1
6	F	82	THR	15.1

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Mol	Chain	Res	Type	RSRZ
10	J	51	LEU	15.1
2	B	504	ARG	15.1
7	G	167	TYR	15.0
2	B	328	GLU	14.9
2	B	642	ASP	14.8
6	F	75	PRO	14.8
7	G	117	GLN	14.8
11	K	79	GLU	14.7
2	B	285	ILE	14.7
1	A	738	LYS	14.7
2	B	278	GLN	14.7
2	B	724	ASP	14.6
1	A	540	PHE	14.5
2	B	1210	MET	14.5
2	B	502	ILE	14.4
7	G	74	TYR	14.4
1	A	1315	GLU	14.4
12	L	51	CYS	14.4
1	A	1163	ILE	14.4
7	G	16	SER	14.3
7	G	40	GLY	14.3
4	D	150	ASN	14.2
2	B	570	VAL	14.2
1	A	1390	ASN	14.2
5	E	84	ASP	14.1
2	B	68	THR	14.1
1	A	382	PRO	14.1
2	B	411	PRO	14.1
2	B	97	VAL	14.1
1	A	179	LEU	14.1
8	H	81	PRO	14.1
1	A	583	PRO	14.0
1	A	558	GLY	14.0
4	D	162	ALA	14.0
10	J	45	CYS	14.0
11	K	67	PHE	13.9
9	I	53	GLY	13.9
2	B	837	ASP	13.9
1	A	1216	ILE	13.9
6	F	154	ASP	13.9
2	B	192	LEU	13.9
9	I	110	PHE	13.9

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Mol	Chain	Res	Type	RSRZ
2	B	371	GLU	13.8
5	E	85	GLU	13.8
2	B	592	ASN	13.8
7	G	27	LYS	13.7
1	A	1231	ASP	13.6
1	A	1233	ASP	13.6
2	B	798	TYR	13.6
1	A	736	ASN	13.6
8	H	135	LEU	13.6
5	E	139	ALA	13.5
1	A	282	ASN	13.5
7	G	12	THR	13.5
1	A	672	ASP	13.4
1	A	1085	HIS	13.4
2	B	61	ASP	13.4
2	B	277	LYS	13.3
1	A	1298	TYR	13.3
5	E	5	ASN	13.3
1	A	791	ASP	13.3
1	A	1162	VAL	13.3
4	D	219	THR	13.3
7	G	52	ASP	13.2
11	K	9	LEU	13.2
1	A	767	GLN	13.2
2	B	725	PRO	13.2
7	G	55	ASP	13.2
7	G	22	MET	13.2
11	K	2	ASN	13.1
1	A	1324	PRO	13.1
3	C	131	HIS	13.1
13	S	169	GLN	13.1
3	C	75	MET	13.1
2	B	206	ASN	13.1
5	E	53	PRO	13.0
10	J	50	ILE	13.0
7	G	81	PRO	13.0
2	B	292	ILE	13.0
4	D	125	SER	13.0
10	J	10	CYS	13.0
13	S	153	LEU	12.9
1	A	786	HIS	12.9
2	B	919	SER	12.9

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Mol	Chain	Res	Type	RSRZ
10	J	13	VAL	12.8
13	S	171	ILE	12.8
4	D	122	GLU	12.8
6	F	130	ILE	12.8
8	H	49	VAL	12.8
3	C	203	GLN	12.8
2	B	529	GLU	12.8
2	B	64	CYS	12.7
1	A	1333	ILE	12.7
1	A	285	PRO	12.7
8	H	109	LYS	12.7
2	B	747	MET	12.7
8	H	7	ASP	12.7
6	F	112	GLU	12.7
2	B	759	PRO	12.7
2	B	542	MET	12.7
1	A	1377	THR	12.7
1	A	358	ASN	12.6
4	D	144	THR	12.6
2	B	1169	MET	12.6
2	B	26	THR	12.5
2	B	736	THR	12.4
2	B	698	GLU	12.4
1	A	525	GLN	12.4
1	A	1210	GLY	12.4
2	B	324	ILE	12.4
2	B	614	SER	12.3
6	F	108	PHE	12.3
1	A	1105	LEU	12.3
2	B	812	LEU	12.3
2	B	524	PRO	12.3
5	E	126	SER	12.3
6	F	93	ILE	12.3
1	A	670	ILE	12.3
2	B	722	ASP	12.2
10	J	40	GLY	12.2
4	D	142	LYS	12.2
2	B	937	ALA	12.2
12	L	63	ARG	12.2
5	E	7	ARG	12.1
1	A	234	MET	12.1
1	A	302	THR	12.1

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Mol	Chain	Res	Type	RSRZ
1	A	853	ASP	12.1
5	E	38	PRO	12.1
1	A	549	MET	12.1
2	B	65	GLU	12.1
1	A	362	ASP	12.0
7	G	24	GLN	12.0
7	G	108	VAL	12.0
5	E	49	SER	12.0
1	A	1228	TRP	11.9
1	A	1230	GLU	11.9
2	B	297	ILE	11.9
5	E	50	MET	11.9
1	A	781	ASP	11.8
2	B	768	THR	11.8
4	D	133	THR	11.8
3	C	88	CYS	11.8
4	D	215	SER	11.8
1	A	815	PHE	11.8
11	K	64	GLU	11.8
1	A	400	PRO	11.8
1	A	909	ASP	11.8
1	A	266	LEU	11.8
1	A	1124	HIS	11.7
3	C	262	LEU	11.7
6	F	110	ASP	11.7
2	B	95	ILE	11.7
11	K	92	ASN	11.7
2	B	96	TYR	11.7
3	C	125	MET	11.7
1	A	1421	CYS	11.7
1	A	4	GLN	11.6
2	B	1052	VAL	11.6
9	I	83	ASN	11.6
1	A	538	ASP	11.6
1	A	820	GLY	11.6
3	C	204	SER	11.6
3	C	256	ALA	11.6
5	E	104	ASN	11.5
2	B	305	VAL	11.5
7	G	47	CYS	11.5
1	A	728	LYS	11.5
2	B	369	GLY	11.5

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Mol	Chain	Res	Type	RSRZ
1	A	239	LEU	11.5
5	E	149	LEU	11.5
2	B	251	ILE	11.5
9	I	10	CYS	11.5
2	B	547	VAL	11.5
1	A	600	PRO	11.5
1	A	52	GLY	11.4
1	A	758	ILE	11.4
2	B	123	THR	11.4
3	C	72	LEU	11.4
3	C	192	TRP	11.4
10	J	39	LEU	11.4
13	S	234	LYS	11.4
2	B	802	PRO	11.4
1	A	1082	ASN	11.4
3	C	95	CYS	11.4
9	I	118	ARG	11.4
1	A	231	PRO	11.3
1	A	110	CYS	11.3
8	H	136	LYS	11.3
7	G	19	GLY	11.3
2	B	763	GLN	11.3
5	E	69	ILE	11.3
1	A	1028	THR	11.2
1	A	94	GLY	11.2
4	D	140	ASP	11.2
1	A	978	PRO	11.2
2	B	678	GLU	11.2
2	B	613	VAL	11.2
1	A	959	ASN	11.2
3	C	60	ASP	11.2
2	B	199	MET	11.1
4	D	164	ILE	11.1
1	A	1200	ALA	11.1
2	B	183	GLU	11.1
1	A	70	CYS	11.1
1	A	755	PHE	11.1
2	B	900	ALA	11.1
2	B	224	GLN	11.1
1	A	1317	MET	11.0
2	B	752	ALA	11.0
2	B	317	CYS	11.0

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Mol	Chain	Res	Type	RSRZ
2	B	329	THR	11.0
2	B	514	LEU	11.0
3	C	29	MET	11.0
8	H	58	THR	11.0
5	E	13	TRP	11.0
13	S	178	ILE	11.0
2	B	24	PRO	11.0
7	G	105	PRO	11.0
5	E	146	HIS	10.9
11	K	85	ASP	10.9
13	S	163	GLU	10.9
13	S	180	SER	10.9
1	A	450	LEU	10.9
1	A	1157	ASP	10.9
2	B	188	ASP	10.9
1	A	930	ASP	10.8
1	A	1074	GLU	10.8
2	B	433	GLN	10.8
3	C	253	LYS	10.8
1	A	61	ILE	10.8
2	B	1104	HIS	10.8
4	D	200	ASN	10.8
1	A	396	PRO	10.7
1	A	615	GLY	10.7
13	S	262	GLU	10.7
2	B	248	SER	10.7
3	C	130	GLY	10.7
1	A	974	ASP	10.7
7	G	26	LEU	10.7
12	L	62	LYS	10.7
1	A	569	LYS	10.7
2	B	571	PRO	10.7
11	K	4	PRO	10.6
1	A	1048	ASN	10.6
1	A	557	ASP	10.6
1	A	75	ASN	10.6
10	J	58	GLU	10.6
5	E	12	LEU	10.6
2	B	456	GLY	10.6
1	A	290	GLU	10.6
6	F	139	PRO	10.6
5	E	39	LEU	10.5

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Mol	Chain	Res	Type	RSRZ
2	B	787	VAL	10.5
8	H	19	ARG	10.5
1	A	480	ALA	10.5
1	A	1138	ILE	10.5
2	B	831	SER	10.5
1	A	1295	THR	10.5
11	K	13	GLY	10.5
2	B	399	ASP	10.5
7	G	123	ALA	10.5
3	C	191	TYR	10.5
1	A	953	ASN	10.5
1	A	656	TRP	10.5
1	A	678	GLU	10.5
2	B	304	ASP	10.4
1	A	288	ALA	10.4
2	B	218	SER	10.4
2	B	167	ILE	10.4
1	A	970	THR	10.4
2	B	1047	PHE	10.4
2	B	593	PRO	10.4
1	A	476	SER	10.4
12	L	33	GLU	10.4
11	K	29	ASN	10.4
2	B	1195	HIS	10.4
3	C	212	PRO	10.3
2	B	774	GLY	10.3
8	H	88	SER	10.3
2	B	1185	CYS	10.3
7	G	126	ASN	10.3
2	B	20	ASP	10.3
1	A	873	MET	10.3
2	B	611	PRO	10.2
1	A	7	SER	10.2
2	B	869	SER	10.2
2	B	503	GLY	10.2
6	F	77	ASP	10.2
9	I	106	CYS	10.2
1	A	826	ASP	10.2
13	S	209	LYS	10.2
2	B	315	LYS	10.2
9	I	116	ASN	10.2
13	S	282	TYR	10.1

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Mol	Chain	Res	Type	RSRZ
1	A	717	ASN	10.1
5	E	140	LEU	10.1
9	I	55	THR	10.1
2	B	1038	SER	10.1
1	A	178	GLY	10.1
2	B	712	PRO	10.1
1	A	438	ASP	10.1
1	A	1439	GLY	10.1
5	E	19	VAL	10.1
2	B	452	THR	10.1
3	C	10	ILE	10.1
5	E	143	ASN	10.1
1	A	854	ASN	10.1
5	E	124	VAL	10.0
5	E	16	PHE	10.0
2	B	975	GLN	10.0
9	I	32	CYS	10.0
1	A	949	ASP	10.0
3	C	110	THR	10.0
13	S	148	LEU	10.0
1	A	425	GLN	10.0
2	B	790	ASP	10.0
2	B	730	ARG	9.9
4	D	218	GLU	9.9
7	G	35	GLU	9.9
5	E	173	SER	9.9
11	K	14	GLU	9.9
3	C	33	LEU	9.9
5	E	40	GLU	9.9
1	A	118	HIS	9.9
13	S	167	PRO	9.9
3	C	17	ASN	9.9
3	C	190	ASP	9.9
2	B	356	LEU	9.9
13	S	260	THR	9.8
7	G	106	MET	9.8
3	C	6	PRO	9.8
12	L	39	SER	9.8
9	I	115	LYS	9.8
1	A	1154	TYR	9.8
1	A	565	ILE	9.8
9	I	29	CYS	9.8

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Mol	Chain	Res	Type	RSRZ
1	A	1255	GLU	9.8
1	A	1084	PHE	9.7
2	B	347	LYS	9.7
2	B	699	GLU	9.7
1	A	1001	ARG	9.7
1	A	1235	LYS	9.7
2	B	170	LEU	9.7
1	A	43	GLU	9.7
1	A	199	LEU	9.7
2	B	412	LEU	9.7
4	D	195	ILE	9.7
1	A	383	TYR	9.7
1	A	1325	THR	9.6
1	A	1361	SER	9.6
2	B	1124	ARG	9.6
1	A	1090	ALA	9.6
1	A	1208	THR	9.6
1	A	1059	HIS	9.6
5	E	159	ASP	9.6
13	S	224	THR	9.6
9	I	103	CYS	9.6
3	C	118	LEU	9.6
8	H	17	PRO	9.6
2	B	401	PHE	9.6
1	A	707	GLY	9.6
1	A	1382	THR	9.5
13	S	193	ALA	9.5
1	A	745	GLN	9.5
4	D	186	ASP	9.5
1	A	694	THR	9.5
2	B	843	GLN	9.5
7	G	13	LEU	9.5
1	A	859	SER	9.5
1	A	1359	ASP	9.5
2	B	1123	SER	9.5
3	C	92	CYS	9.5
6	F	126	ALA	9.5
11	K	22	ASP	9.5
1	A	877	HIS	9.4
1	A	310	GLY	9.4
2	B	168	GLY	9.4
1	A	41	MET	9.4

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Mol	Chain	Res	Type	RSRZ
2	B	382	ILE	9.4
1	A	481	ASP	9.4
1	A	680	THR	9.4
1	A	801	GLU	9.3
11	K	86	ALA	9.3
1	A	887	GLY	9.3
7	G	51	TYR	9.3
1	A	436	ILE	9.3
12	L	50	ASP	9.3
5	E	153	HIS	9.3
3	C	208	GLU	9.3
7	G	155	SER	9.3
2	B	905	VAL	9.3
1	A	6	TYR	9.3
1	A	218	ASP	9.3
2	B	576	ASP	9.3
2	B	552	MET	9.3
6	F	84	TYR	9.2
3	C	123	ASN	9.2
4	D	149	THR	9.2
2	B	819	ALA	9.2
1	A	62	ASP	9.2
1	A	54	ASN	9.2
3	C	189	THR	9.2
13	S	217	LYS	9.2
6	F	119	ARG	9.2
1	A	23	SER	9.2
8	H	134	ASN	9.1
6	F	149	GLU	9.1
13	S	203	TYR	9.1
2	B	364	ILE	9.1
1	A	1072	ILE	9.1
7	G	7	LEU	9.1
1	A	695	LYS	9.1
2	B	449	ASN	9.1
1	A	1111	MET	9.1
7	G	25	TYR	9.0
1	A	1113	THR	9.0
5	E	152	LYS	9.0
13	S	289	ALA	9.0
1	A	1145	SER	9.0
2	B	180	TYR	9.0

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Mol	Chain	Res	Type	RSRZ
3	C	3	GLU	9.0
5	E	204	THR	9.0
10	J	15	GLY	9.0
11	K	89	ASN	9.0
1	A	409	SER	9.0
2	B	298	LEU	9.0
9	I	93	LYS	9.0
1	A	174	ILE	9.0
1	A	843	LYS	9.0
3	C	67	LEU	9.0
2	B	427	ASP	9.0
1	A	494	SER	9.0
1	A	807	GLY	8.9
2	B	646	LEU	8.9
1	A	276	LEU	8.9
1	A	369	SER	8.9
1	A	919	ILE	8.9
5	E	2	ASP	8.9
2	B	862	GLN	8.9
1	A	475	THR	8.9
13	S	220	ASN	8.9
9	I	39	GLY	8.9
2	B	250	PHE	8.9
2	B	198	ASP	8.9
3	C	134	ILE	8.8
1	A	905	ASP	8.8
2	B	746	SER	8.8
3	C	210	GLU	8.8
1	A	129	LYS	8.8
3	C	86	CYS	8.8
1	A	1010	ALA	8.8
2	B	106	ASP	8.8
4	D	193	THR	8.8
1	A	113	LEU	8.8
9	I	59	VAL	8.8
9	I	44	TYR	8.8
5	E	96	PHE	8.8
7	G	20	PRO	8.8
1	A	1347	ALA	8.7
2	B	569	TYR	8.7
1	A	1242	VAL	8.7
1	A	1453	TYR	8.7

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Mol	Chain	Res	Type	RSRZ
1	A	392	VAL	8.7
11	K	11	LEU	8.7
2	B	43	LEU	8.7
13	S	214	LEU	8.7
1	A	419	LYS	8.7
9	I	4	PHE	8.7
11	K	40	HIS	8.7
2	B	499	ASN	8.7
1	A	1076	ALA	8.7
1	A	829	VAL	8.7
5	E	74	ASP	8.7
9	I	60	GLN	8.7
2	B	325	GLN	8.7
13	S	257	GLN	8.7
2	B	457	LEU	8.6
2	B	791	THR	8.6
3	C	186	LEU	8.6
1	A	732	LEU	8.6
13	S	273	LYS	8.6
2	B	744	HIS	8.6
10	J	6	ARG	8.6
9	I	64	SER	8.6
1	A	1316	VAL	8.6
2	B	520	GLY	8.6
13	S	202	ILE	8.6
2	B	713	ALA	8.6
8	H	86	ASP	8.6
13	S	261	ILE	8.5
13	S	144	TYR	8.5
1	A	1055	ARG	8.5
1	A	673	GLY	8.5
3	C	180	TYR	8.5
7	G	149	GLY	8.5
1	A	209	ASN	8.5
1	A	589	GLN	8.5
11	K	109	TRP	8.5
2	B	917	PRO	8.4
2	B	1149	GLU	8.4
1	A	1203	ASN	8.4
1	A	1264	GLU	8.4
4	D	181	GLY	8.4
1	A	109	HIS	8.4

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Mol	Chain	Res	Type	RSRZ
2	B	221	ASN	8.4
1	A	275	SER	8.4
11	K	59	ALA	8.4
1	A	1077	THR	8.4
1	A	1040	GLN	8.4
11	K	113	THR	8.4
2	B	534	GLY	8.4
7	G	138	THR	8.3
13	S	221	GLY	8.3
2	B	806	THR	8.3
1	A	649	ILE	8.3
10	J	16	ASP	8.3
1	A	1341	ILE	8.3
2	B	105	SER	8.3
13	S	168	PRO	8.3
8	H	47	PHE	8.3
2	B	517	THR	8.3
7	G	45	ILE	8.3
2	B	414	ALA	8.3
2	B	859	TYR	8.3
13	S	251	GLN	8.3
1	A	284	ALA	8.3
10	J	3	VAL	8.3
1	A	397	ASN	8.3
1	A	989	GLY	8.3
2	B	1114	LEU	8.3
2	B	1125	ASP	8.2
8	H	110	ASP	8.2
7	G	48	VAL	8.2
1	A	1110	ASN	8.2
2	B	437	GLU	8.2
13	S	208	SER	8.2
3	C	214	ASN	8.2
3	C	34	ARG	8.2
1	A	722	LEU	8.2
2	B	658	ILE	8.2
2	B	435	THR	8.2
1	A	1353	TYR	8.2
1	A	1006	ILE	8.2
11	K	112	GLN	8.2
9	I	86	PHE	8.2
2	B	396	ASP	8.2

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Mol	Chain	Res	Type	RSRZ
4	D	198	LEU	8.2
6	F	97	ARG	8.2
12	L	25	ALA	8.2
8	H	102	TYR	8.2
1	A	1017	LEU	8.2
2	B	284	ILE	8.2
1	A	1213	GLY	8.1
2	B	856	PHE	8.1
1	A	69	THR	8.1
1	A	1448	GLU	8.1
2	B	657	HIS	8.1
1	A	77	CYS	8.1
2	B	873	THR	8.1
13	S	218	ILE	8.1
11	K	49	GLU	8.1
1	A	833	GLU	8.0
1	A	1000	LEU	8.0
2	B	29	ASP	8.0
3	C	249	ASP	8.0
6	F	143	PHE	8.0
3	C	91	HIS	8.0
1	A	601	LYS	8.0
2	B	939	THR	8.0
1	A	792	TYR	8.0
8	H	76	THR	8.0
3	C	144	ILE	8.0
1	A	1219	THR	8.0
1	A	378	GLU	8.0
10	J	46	CYS	8.0
2	B	875	GLU	8.0
1	A	168	GLY	8.0
2	B	302	CYS	8.0
1	A	1116	LEU	8.0
2	B	849	GLY	8.0
3	C	5	GLY	8.0
1	A	291	GLU	8.0
2	B	622	LYS	8.0
2	B	1077	THR	8.0
12	L	66	GLN	8.0
2	B	346	GLU	8.0
1	A	274	ILE	7.9
7	G	164	LYS	7.9

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Mol	Chain	Res	Type	RSRZ
13	S	160	LEU	7.9
1	A	714	PHE	7.9
2	B	314	LEU	7.9
1	A	1215	ARG	7.9
1	A	1374	VAL	7.9
1	A	286	HIS	7.9
13	S	164	SER	7.9
1	A	862	ASN	7.9
13	S	196	LYS	7.9
2	B	219	ALA	7.9
9	I	90	GLN	7.8
1	A	780	VAL	7.8
1	A	903	ASN	7.8
2	B	114	PRO	7.8
2	B	1156	ASP	7.8
3	C	176	ILE	7.8
1	A	261	ASP	7.8
1	A	5	GLN	7.8
2	B	619	ILE	7.8
2	B	1050	ILE	7.8
7	G	30	LEU	7.8
1	A	201	VAL	7.8
1	A	1012	ARG	7.8
12	L	34	CYS	7.8
1	A	834	THR	7.8
2	B	448	ILE	7.8
11	K	15	GLY	7.8
1	A	1292	PRO	7.8
2	B	312	GLU	7.8
1	A	472	LEU	7.8
1	A	1161	THR	7.8
11	K	54	ARG	7.8
2	B	1063	GLY	7.7
3	C	209	TYR	7.7
2	B	830	TYR	7.7
2	B	417	PHE	7.7
1	A	965	GLN	7.7
2	B	1202	LEU	7.7
1	A	971	PHE	7.7
2	B	754	SER	7.7
10	J	52	THR	7.7
1	A	1277	GLU	7.7

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Mol	Chain	Res	Type	RSRZ
2	B	1189	ILE	7.7
1	A	580	VAL	7.7
2	B	647	GLY	7.7
4	D	184	ALA	7.7
1	A	1127	ASP	7.7
1	A	37	PHE	7.6
1	A	1065	GLY	7.6
1	A	735	VAL	7.6
7	G	34	VAL	7.6
2	B	1216	LEU	7.6
3	C	222	LYS	7.6
9	I	48	LEU	7.6
1	A	1122	PRO	7.6
1	A	99	ILE	7.6
1	A	705	LYS	7.6
2	B	961	LEU	7.6
11	K	110	ASN	7.6
2	B	288	ALA	7.5
1	A	413	ILE	7.5
10	J	27	GLU	7.5
6	F	94	LEU	7.5
3	C	63	ILE	7.5
2	B	665	GLU	7.5
2	B	621	GLU	7.5
8	H	50	ALA	7.5
8	H	32	THR	7.5
5	E	158	SER	7.5
1	A	148	CYS	7.5
1	A	1397	LEU	7.5
2	B	1031	LEU	7.5
6	F	102	SER	7.5
10	J	36	LEU	7.5
2	B	308	TRP	7.5
8	H	28	ALA	7.5
1	A	935	GLN	7.5
1	A	167	CYS	7.5
5	E	106	GLN	7.5
2	B	429	PHE	7.4
3	C	62	PHE	7.4
2	B	1035	ALA	7.4
2	B	773	MET	7.4
1	A	1101	LEU	7.4

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Mol	Chain	Res	Type	RSRZ
1	A	1130	GLN	7.4
9	I	75	CYS	7.4
1	A	347	PHE	7.4
8	H	54	SER	7.4
2	B	350	GLN	7.4
11	K	98	LEU	7.4
1	A	1184	SER	7.4
9	I	40	SER	7.4
1	A	986	ILE	7.4
4	D	185	CYS	7.4
1	A	742	ASN	7.4
1	A	992	ASP	7.4
2	B	332	ASP	7.4
2	B	652	LYS	7.4
5	E	145	THR	7.4
7	G	56	ILE	7.4
6	F	104	ASN	7.4
1	A	709	THR	7.4
1	A	1205	LYS	7.4
11	K	53	ASP	7.4
1	A	1269	GLU	7.3
1	A	287	HIS	7.3
2	B	42	GLY	7.3
2	B	120	ARG	7.3
1	A	683	ILE	7.3
2	B	1138	MET	7.3
1	A	1132	LYS	7.3
4	D	161	GLY	7.3
2	B	531	GLN	7.3
2	B	1147	LEU	7.3
7	G	50	ASP	7.3
6	F	131	PRO	7.3
1	A	1079	MET	7.2
2	B	934	LYS	7.2
13	S	298	THR	7.2
6	F	123	LYS	7.2
8	H	118	PHE	7.2
1	A	1232	ASN	7.2
2	B	864	LYS	7.2
2	B	1221	SER	7.2
2	B	1136	ASP	7.2
4	D	191	ALA	7.2

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Mol	Chain	Res	Type	RSRZ
5	E	32	GLN	7.2
1	A	1173	HIS	7.2
8	H	83	GLN	7.2
4	D	167	LEU	7.2
1	A	491	VAL	7.2
1	A	1435	PRO	7.2
2	B	256	VAL	7.2
2	B	299	GLU	7.2
3	C	244	VAL	7.2
1	A	298	PHE	7.2
2	B	389	ALA	7.2
1	A	447	GLN	7.2
1	A	969	GLN	7.2
2	B	455	SER	7.2
5	E	179	GLN	7.2
5	E	184	VAL	7.2
7	G	43	GLY	7.2
9	I	68	LEU	7.2
2	B	739	THR	7.2
13	S	267	ASP	7.1
1	A	1429	ILE	7.1
2	B	912	ILE	7.1
2	B	751	VAL	7.1
1	A	1052	GLN	7.1
7	G	75	ARG	7.1
3	C	78	GLU	7.1
13	S	266	THR	7.1
1	A	645	LEU	7.1
10	J	17	LYS	7.1
2	B	559	SER	7.1
2	B	181	LEU	7.1
4	D	199	ASN	7.1
2	B	579	ARG	7.1
1	A	1131	ALA	7.1
1	A	860	LEU	7.1
2	B	627	PHE	7.1
1	A	1143	LEU	7.1
6	F	127	GLU	7.1
1	A	1166	ASP	7.1
1	A	756	ILE	7.1
1	A	977	LYS	7.1
2	B	99	LYS	7.1

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Mol	Chain	Res	Type	RSRZ
1	A	677	ARG	7.0
13	S	204	SER	7.0
3	C	58	LEU	7.0
3	C	255	VAL	7.0
5	E	101	GLN	7.0
4	D	204	ASP	7.0
12	L	44	ASP	7.0
9	I	38	ALA	7.0
10	J	5	VAL	7.0
6	F	92	ARG	7.0
2	B	178	ASN	7.0
2	B	233	PRO	7.0
2	B	1036	ALA	7.0
13	S	225	PRO	7.0
1	A	1342	GLU	7.0
10	J	57	ILE	7.0
7	G	11	ILE	7.0
1	A	698	GLN	7.0
13	S	179	GLU	7.0
10	J	20	SER	7.0
2	B	373	ARG	7.0
11	K	3	ALA	7.0
13	S	238	PRO	6.9
2	B	820	GLY	6.9
3	C	165	LYS	6.9
1	A	499	ALA	6.9
5	E	189	GLY	6.9
5	E	99	HIS	6.9
1	A	629	LEU	6.9
2	B	280	ILE	6.9
12	L	31	CYS	6.9
1	A	226	GLU	6.9
2	B	618	ASP	6.9
2	B	1166	CYS	6.9
11	K	8	GLU	6.9
2	B	811	TYR	6.9
2	B	493	SER	6.9
1	A	309	ALA	6.9
3	C	243	VAL	6.9
1	A	185	TRP	6.9
1	A	1344	GLY	6.9
2	B	22	SER	6.9

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Mol	Chain	Res	Type	RSRZ
2	B	226	PHE	6.9
2	B	272	THR	6.9
1	A	31	SER	6.9
4	D	203	SER	6.9
8	H	113	ALA	6.9
2	B	946	ASN	6.9
2	B	1026	LEU	6.9
5	E	18	THR	6.9
8	H	117	SER	6.9
2	B	390	LEU	6.8
1	A	105	CYS	6.8
2	B	232	SER	6.8
3	C	236	GLY	6.8
2	B	197	PHE	6.8
2	B	891	ASP	6.8
5	E	144	ILE	6.8
4	D	176	GLU	6.8
1	A	1225	PHE	6.8
2	B	887	HIS	6.8
11	K	76	GLN	6.8
1	A	790	ASP	6.8
1	A	1376	THR	6.8
2	B	832	GLY	6.8
1	A	370	ILE	6.8
1	A	821	ARG	6.8
7	G	64	THR	6.8
1	A	545	GLN	6.8
2	B	209	GLU	6.8
3	C	166	GLU	6.8
2	B	283	VAL	6.8
1	A	823	GLY	6.7
1	A	727	ASP	6.7
1	A	1403	GLU	6.7
2	B	58	THR	6.7
1	A	164	ARG	6.7
3	C	250	THR	6.7
4	D	173	HIS	6.7
8	H	120	GLY	6.7
10	J	19	GLU	6.7
1	A	932	GLU	6.7
1	A	1042	PHE	6.7
2	B	1137	CYS	6.7

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Mol	Chain	Res	Type	RSRZ
1	A	1430	LEU	6.7
1	A	1199	ARG	6.7
2	B	878	GLN	6.7
1	A	1286	LYS	6.7
9	I	82	GLU	6.7
1	A	1394	THR	6.7
2	B	633	VAL	6.7
12	L	46	VAL	6.6
1	A	1371	LEU	6.6
3	C	258	ILE	6.6
8	H	52	GLN	6.6
1	A	1058	VAL	6.6
2	B	92	PHE	6.6
11	K	7	PHE	6.6
1	A	1022	LEU	6.6
2	B	394	ASP	6.6
2	B	1066	SER	6.6
2	B	880	THR	6.6
1	A	514	PRO	6.6
1	A	1302	PRO	6.6
2	B	867	GLY	6.6
1	A	356	ASP	6.6
1	A	150	THR	6.6
2	B	916	THR	6.6
7	G	99	PHE	6.6
1	A	924	LYS	6.6
2	B	1183	LYS	6.6
10	J	4	PRO	6.6
13	S	141	THR	6.6
1	A	654	ASN	6.6
9	I	36	GLU	6.6
3	C	237	SER	6.6
1	A	999	VAL	6.6
1	A	144	THR	6.5
1	A	578	LEU	6.5
5	E	185	ALA	6.5
1	A	774	ARG	6.5
6	F	122	MET	6.5
7	G	93	SER	6.5
1	A	1109	LYS	6.5
1	A	595	THR	6.5
5	E	123	LEU	6.5

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Mol	Chain	Res	Type	RSRZ
1	A	162	VAL	6.5
2	B	383	ASN	6.5
2	B	1153	GLU	6.5
2	B	1082	MET	6.5
1	A	795	GLU	6.5
3	C	65	HIS	6.5
1	A	839	ARG	6.5
2	B	1034	VAL	6.5
1	A	692	ASP	6.5
9	I	65	ASP	6.5
2	B	631	GLY	6.5
2	B	125	SER	6.5
2	B	1133	MET	6.5
4	D	165	GLN	6.5
13	S	207	ILE	6.5
3	C	16	ASP	6.5
1	A	172	PRO	6.5
5	E	68	SER	6.4
1	A	1385	THR	6.4
1	A	576	GLN	6.4
1	A	386	ASP	6.4
1	A	408	ASP	6.4
5	E	132	ILE	6.4
2	B	962	LYS	6.4
6	F	74	ILE	6.4
9	I	89	GLN	6.4
7	G	141	SER	6.4
1	A	660	ASN	6.4
8	H	41	ASP	6.4
11	K	82	ASP	6.4
1	A	726	ARG	6.4
3	C	198	ALA	6.4
5	E	10	SER	6.4
11	K	45	LEU	6.4
3	C	167	HIS	6.4
2	B	1007	VAL	6.4
1	A	1117	THR	6.4
2	B	103	ASN	6.4
2	B	489	SER	6.4
2	B	311	LEU	6.4
2	B	667	GLN	6.4
4	D	194	LEU	6.4

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Mol	Chain	Res	Type	RSRZ
1	A	68	GLN	6.3
1	A	1387	HIS	6.3
2	B	35	SER	6.3
4	D	220	LEU	6.3
1	A	128	ILE	6.3
1	A	1263	ILE	6.3
11	K	95	ILE	6.3
7	G	32	GLU	6.3
2	B	648	HIS	6.3
3	C	42	PRO	6.3
1	A	1002	GLY	6.3
3	C	219	PHE	6.3
13	S	182	MET	6.3
11	K	91	CYS	6.3
13	S	185	VAL	6.3
1	A	640	GLN	6.3
1	A	771	GLU	6.3
2	B	38	PHE	6.3
2	B	1111	MET	6.3
1	A	806	ARG	6.3
2	B	1100	ASP	6.3
2	B	1182	CYS	6.3
1	A	650	GLN	6.3
2	B	662	MET	6.3
2	B	682	SER	6.3
3	C	241	ASP	6.3
5	E	72	PHE	6.3
1	A	1410	PHE	6.2
10	J	2	ILE	6.2
10	J	63	TYR	6.2
1	A	124	GLN	6.2
1	A	381	THR	6.2
2	B	537	LYS	6.2
5	E	174	GLN	6.2
2	B	323	VAL	6.2
3	C	242	GLN	6.2
12	L	35	SER	6.2
1	A	1141	THR	6.2
1	A	1420	ASP	6.2
1	A	1068	ALA	6.2
1	A	222	LEU	6.2
2	B	651	LEU	6.2

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Mol	Chain	Res	Type	RSRZ
4	D	168	LYS	6.2
2	B	1178	ASN	6.2
7	G	38	CYS	6.2
1	A	86	LEU	6.2
2	B	51	PHE	6.2
1	A	1223	ASP	6.2
10	J	53	HIS	6.2
2	B	918	ILE	6.2
6	F	106	PRO	6.2
13	S	157	TYR	6.1
2	B	109	THR	6.1
1	A	306	ASN	6.1
2	B	863	GLU	6.1
11	K	96	ASN	6.1
1	A	533	LYS	6.1
1	A	1362	TYR	6.1
2	B	615	MET	6.1
7	G	136	VAL	6.1
7	G	166	ASP	6.1
1	A	268	ASP	6.1
3	C	66	ARG	6.1
1	A	241	VAL	6.1
8	H	33	GLN	6.1
13	S	281	TYR	6.1
1	A	176	LYS	6.1
7	G	143	ILE	6.1
2	B	575	PRO	6.1
1	A	9	ALA	6.1
8	H	3	ASN	6.1
13	S	140	ASP	6.1
6	F	146	TRP	6.1
2	B	321	GLY	6.1
5	E	196	VAL	6.1
1	A	503	GLN	6.1
1	A	1373	ASP	6.1
1	A	501	LEU	6.1
6	F	90	ARG	6.1
1	A	1169	ILE	6.0
1	A	1348	LEU	6.0
4	D	119	ARG	6.0
10	J	56	LEU	6.0
1	A	585	GLY	6.0

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Mol	Chain	Res	Type	RSRZ
5	E	148	GLU	6.0
2	B	645	SER	6.0
2	B	598	GLU	6.0
2	B	738	PHE	6.0
1	A	213	HIS	6.0
1	A	805	LEU	6.0
2	B	986	GLN	6.0
5	E	67	GLU	6.0
1	A	891	ALA	6.0
7	G	124	GLY	6.0
7	G	102	GLN	6.0
2	B	734	HIS	6.0
13	S	199	TYR	6.0
1	A	1088	GLY	6.0
2	B	743	ILE	6.0
1	A	1098	VAL	6.0
1	A	55	ASP	6.0
13	S	192	GLU	6.0
7	G	80	LYS	6.0
5	E	100	ILE	6.0
2	B	98	THR	6.0
2	B	760	ASP	6.0
9	I	94	ASP	6.0
3	C	31	ASN	6.0
1	A	941	LYS	6.0
4	D	216	ASN	6.0
1	A	151	ASP	6.0
1	A	837	ILE	6.0
2	B	737	THR	6.0
3	C	112	ASN	5.9
1	A	1067	LEU	5.9
5	E	120	ALA	5.9
1	A	897	TYR	5.9
13	S	139	VAL	5.9
9	I	95	THR	5.9
13	S	254	TYR	5.9
13	S	271	CYS	5.9
1	A	1189	SER	5.9
2	B	235	SER	5.9
13	S	170	SER	5.9
1	A	1019	CYS	5.9
1	A	57	ARG	5.9

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Mol	Chain	Res	Type	RSRZ
2	B	663	ALA	5.9
1	A	526	ASP	5.9
7	G	39	THR	5.9
1	A	175	ARG	5.9
1	A	643	ALA	5.9
6	F	129	LYS	5.9
2	B	380	TYR	5.9
1	A	1123	GLY	5.9
9	I	109	ILE	5.8
3	C	268	ASP	5.8
9	I	54	GLU	5.8
3	C	115	SER	5.8
1	A	1118	VAL	5.8
1	A	882	SER	5.8
2	B	398	ARG	5.8
2	B	1139	ILE	5.8
1	A	335	ARG	5.8
2	B	753	ALA	5.8
11	K	103	THR	5.8
1	A	277	GLU	5.8
4	D	154	PHE	5.8
13	S	136	ASN	5.8
1	A	938	LYS	5.8
11	K	10	PHE	5.8
1	A	130	ASP	5.8
5	E	45	LYS	5.8
11	K	93	SER	5.8
1	A	393	ARG	5.8
1	A	1202	MET	5.8
3	C	102	GLN	5.8
1	A	1207	LEU	5.8
2	B	395	GLN	5.8
3	C	52	GLU	5.8
1	A	448	PRO	5.8
1	A	1197	LEU	5.8
5	E	129	PRO	5.8
2	B	1207	LEU	5.8
3	C	89	GLU	5.8
4	D	153	ARG	5.8
1	A	452	LYS	5.8
1	A	951	GLU	5.8
1	A	939	ASP	5.8

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Mol	Chain	Res	Type	RSRZ
9	I	70	ARG	5.7
12	L	70	ARG	5.7
3	C	70	ILE	5.7
1	A	67	CYS	5.7
1	A	685	GLU	5.7
4	D	197	SER	5.7
1	A	1349	TYR	5.7
13	S	219	ALA	5.7
2	B	467	GLY	5.7
1	A	146	MET	5.7
7	G	57	GLN	5.7
1	A	289	ILE	5.7
2	B	888	GLY	5.7
11	K	28	PRO	5.7
11	K	105	PHE	5.7
1	A	297	GLN	5.7
8	H	138	GLU	5.7
3	C	68	GLY	5.7
2	B	131	ASP	5.7
12	L	38	LEU	5.7
1	A	1364	ASN	5.7
2	B	189	LEU	5.7
1	A	439	ASN	5.7
2	B	1109	GLY	5.7
3	C	199	LYS	5.6
9	I	119	THR	5.6
1	A	116	ASP	5.6
2	B	761	HIS	5.6
2	B	944	THR	5.6
6	F	113	GLY	5.6
2	B	351	TYR	5.6
1	A	783	THR	5.6
10	J	22	LEU	5.6
2	B	998	ASP	5.6
1	A	721	PHE	5.6
2	B	45	SER	5.6
1	A	871	ASP	5.6
2	B	245	GLU	5.6
2	B	249	ARG	5.6
13	S	216	HIS	5.6
1	A	1005	GLU	5.6
1	A	479	ASN	5.6

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Mol	Chain	Res	Type	RSRZ
1	A	484	GLY	5.6
2	B	885	MET	5.6
2	B	548	GLY	5.6
7	G	153	GLN	5.6
8	H	91	ASP	5.6
4	D	163	VAL	5.6
5	E	93	MET	5.6
8	H	20	TYR	5.6
1	A	1412	ALA	5.6
6	F	73	ALA	5.6
1	A	809	THR	5.6
2	B	177	LYS	5.6
1	A	1368	MET	5.6
5	E	182	ASP	5.6
1	A	659	HIS	5.5
9	I	13	MET	5.5
11	K	21	ILE	5.5
2	B	391	ASP	5.5
5	E	11	ARG	5.5
4	D	159	THR	5.5
2	B	933	SER	5.5
2	B	555	ILE	5.5
13	S	158	ASP	5.5
11	K	42	LEU	5.5
1	A	794	PRO	5.5
2	B	374	LYS	5.5
1	A	60	SER	5.5
6	F	147	SER	5.5
7	G	37	SER	5.5
1	A	493	GLN	5.5
11	K	56	VAL	5.5
3	C	261	ALA	5.5
1	A	1176	LEU	5.5
2	B	52	ASN	5.5
8	H	5	LEU	5.5
2	B	785	TYR	5.5
7	G	1	MET	5.5
6	F	105	ALA	5.5
1	A	1104	ILE	5.4
1	A	1218	GLN	5.4
1	A	1229	SER	5.4
2	B	1217	TYR	5.4

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Mol	Chain	Res	Type	RSRZ
2	B	1175	LEU	5.4
2	B	868	MET	5.4
1	A	710	LEU	5.4
1	A	238	CYS	5.4
2	B	898	LEU	5.4
1	A	573	SER	5.4
7	G	62	LEU	5.4
1	A	440	ASP	5.4
1	A	923	LEU	5.4
1	A	10	PRO	5.4
2	B	562	GLY	5.4
1	A	793	SER	5.4
1	A	946	VAL	5.4
2	B	419	THR	5.4
1	A	183	GLY	5.4
2	B	861	ASP	5.4
1	A	883	LEU	5.4
2	B	996	ARG	5.4
1	A	885	THR	5.4
1	A	937	VAL	5.4
2	B	516	ASN	5.4
2	B	890	TYR	5.4
5	E	105	PHE	5.4
5	E	4	GLU	5.3
2	B	117	ALA	5.3
1	A	1381	LEU	5.3
1	A	904	THR	5.3
1	A	210	ILE	5.3
1	A	1172	LEU	5.3
1	A	995	GLU	5.3
1	A	173	THR	5.3
5	E	195	VAL	5.3
2	B	899	ILE	5.3
2	B	1159	ARG	5.3
3	C	97	VAL	5.3
7	G	42	PHE	5.3
8	H	130	ARG	5.3
1	A	687	LYS	5.3
1	A	665	GLY	5.3
1	A	373	THR	5.3
2	B	229	ALA	5.3
3	C	53	THR	5.3

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Mol	Chain	Res	Type	RSRZ
1	A	321	PRO	5.3
13	S	228	LEU	5.3
1	A	973	ILE	5.3
2	B	418	LYS	5.3
1	A	519	PRO	5.2
4	D	120	GLU	5.2
2	B	715	ALA	5.2
2	B	779	GLY	5.2
3	C	171	GLY	5.2
4	D	171	GLY	5.2
2	B	413	LEU	5.2
5	E	27	GLY	5.2
2	B	1180	PHE	5.2
1	A	8	SER	5.2
2	B	983	ARG	5.2
1	A	1128	GLN	5.2
2	B	402	GLY	5.2
3	C	223	ALA	5.2
5	E	63	ASN	5.2
1	A	918	GLU	5.2
2	B	807	ARG	5.2
7	G	3	PHE	5.2
7	G	61	ILE	5.2
1	A	1378	GLN	5.2
8	H	93	TYR	5.2
1	A	731	ARG	5.2
1	A	816	HIS	5.2
1	A	1319	VAL	5.2
1	A	827	THR	5.2
1	A	418	SER	5.2
7	G	14	HIS	5.2
1	A	449	SER	5.2
2	B	196	PRO	5.2
2	B	527	THR	5.1
6	F	78	GLN	5.1
8	H	18	GLY	5.1
1	A	96	ILE	5.1
1	A	426	LEU	5.1
1	A	1331	SER	5.1
1	A	1400	CYS	5.1
2	B	988	GLY	5.1
1	A	95	PHE	5.1

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Mol	Chain	Res	Type	RSRZ
2	B	1145	SER	5.1
7	G	58	ARG	5.1
9	I	114	GLN	5.1
2	B	1023	VAL	5.1
1	A	235	ILE	5.1
13	S	154	LYS	5.1
1	A	831	THR	5.1
7	G	127	PRO	5.1
2	B	1017	ILE	5.1
1	A	42	ASP	5.1
1	A	80	HIS	5.1
1	A	511	ILE	5.1
1	A	71	GLN	5.1
1	A	1060	PRO	5.1
1	A	3	GLY	5.1
1	A	85	ASP	5.1
1	A	1013	ASP	5.1
9	I	117	LYS	5.1
1	A	1402	PHE	5.1
2	B	660	LYS	5.1
1	A	184	SER	5.1
2	B	742	GLU	5.1
7	G	54	ILE	5.1
1	A	346	ASP	5.0
1	A	1428	VAL	5.0
2	B	963	PHE	5.0
9	I	87	GLN	5.0
1	A	1343	ALA	5.0
2	B	710	LEU	5.0
3	C	216	GLY	5.0
4	D	182	SER	5.0
13	S	258	GLY	5.0
1	A	529	CYS	5.0
1	A	149	GLU	5.0
1	A	424	ILE	5.0
2	B	617	ARG	5.0
2	B	1029	CYS	5.0
11	K	87	LEU	5.0
1	A	917	SER	5.0
2	B	1022	THR	5.0
2	B	1204	PHE	5.0
2	B	953	LEU	5.0

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Mol	Chain	Res	Type	RSRZ
2	B	1061	GLU	5.0
13	S	243	GLN	5.0
1	A	1311	VAL	5.0
2	B	851	PHE	5.0
3	C	168	ALA	5.0
1	A	993	LEU	5.0
2	B	1206	GLU	5.0
1	A	675	THR	5.0
10	J	44	TYR	5.0
2	B	538	ASN	5.0
7	G	156	SER	5.0
2	B	59	LEU	5.0
3	C	135	GLN	5.0
1	A	1388	GLY	5.0
1	A	1258	HIS	5.0
4	D	116	SER	5.0
1	A	136	ALA	5.0
3	C	80	LEU	5.0
8	H	84	ALA	5.0
9	I	73	ARG	5.0
1	A	1261	LYS	5.0
11	K	46	ILE	5.0
3	C	4	GLU	5.0
13	S	252	ASN	4.9
1	A	220	THR	4.9
1	A	530	GLY	4.9
1	A	957	PRO	4.9
1	A	1038	THR	4.9
1	A	1066	VAL	4.9
10	J	7	CYS	4.9
2	B	132	VAL	4.9
1	A	669	THR	4.9
1	A	211	PHE	4.9
1	A	842	VAL	4.9
3	C	51	VAL	4.9
1	A	910	PRO	4.9
2	B	561	TRP	4.9
2	B	594	ALA	4.9
1	A	975	HIS	4.9
13	S	156	LEU	4.9
13	S	187	ASN	4.9
1	A	567	LYS	4.9

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Mol	Chain	Res	Type	RSRZ
2	B	588	GLY	4.9
7	G	114	LEU	4.9
1	A	1425	SER	4.9
2	B	845	SER	4.9
2	B	1205	GLN	4.9
2	B	282	ILE	4.9
2	B	1101	ASP	4.9
1	A	1095	THR	4.9
2	B	1046	PRO	4.9
7	G	128	PRO	4.9
2	B	322	PHE	4.9
7	G	8	SER	4.9
8	H	11	GLN	4.9
1	A	48	ALA	4.9
1	A	125	ALA	4.9
13	S	245	ILE	4.9
1	A	623	GLY	4.9
1	A	1182	GLU	4.9
2	B	1103	ILE	4.9
1	A	1148	ILE	4.9
1	A	835	GLY	4.9
1	A	979	SER	4.9
1	A	1075	PRO	4.9
1	A	1102	LYS	4.9
1	A	1115	SER	4.9
2	B	984	HIS	4.9
2	B	491	THR	4.9
7	G	98	GLY	4.9
2	B	1015	HIS	4.9
1	A	485	ASP	4.8
2	B	835	GLN	4.8
7	G	148	GLU	4.8
2	B	1107	ALA	4.8
4	D	212	LYS	4.8
1	A	1321	GLY	4.8
4	D	213	GLU	4.8
2	B	1058	LEU	4.8
1	A	1144	LYS	4.8
1	A	360	GLU	4.8
1	A	611	GLN	4.8
3	C	50	GLU	4.8
3	C	139	GLY	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	270	LEU	4.8
5	E	128	PRO	4.8
11	K	66	PRO	4.8
13	S	205	ASN	4.8
12	L	40	LEU	4.8
1	A	674	PRO	4.8
8	H	62	SER	4.8
2	B	808	ALA	4.8
1	A	1406	VAL	4.8
1	A	733	ALA	4.8
9	I	69	PRO	4.8
1	A	30	ILE	4.8
9	I	31	THR	4.8
1	A	1427	ASN	4.8
2	B	977	GLY	4.8
2	B	1102	LYS	4.8
9	I	5	ARG	4.8
2	B	367	LEU	4.8
2	B	406	LEU	4.8
1	A	723	ASN	4.8
1	A	245	PRO	4.8
1	A	626	ASN	4.8
2	B	247	GLY	4.8
3	C	259	LEU	4.8
1	A	1449	SER	4.7
2	B	604	ARG	4.7
1	A	785	PRO	4.7
1	A	27	VAL	4.7
2	B	510	LYS	4.7
9	I	50	THR	4.7
1	A	388	LEU	4.7
1	A	787	PHE	4.7
1	A	510	GLN	4.7
1	A	641	VAL	4.7
2	B	700	SER	4.7
7	G	116	PRO	4.7
7	G	60	ARG	4.7
1	A	102	VAL	4.7
6	F	89	GLU	4.7
1	A	784	LEU	4.7
2	B	486	TYR	4.7
1	A	958	VAL	4.7

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Mol	Chain	Res	Type	RSRZ
2	B	1116	ARG	4.7
1	A	206	GLU	4.7
2	B	266	ALA	4.7
1	A	744	LYS	4.7
1	A	729	ALA	4.7
2	B	318	VAL	4.7
2	B	422	LYS	4.7
1	A	336	ILE	4.7
2	B	847	ASP	4.7
1	A	502	SER	4.6
1	A	704	ALA	4.6
1	A	1334	ASP	4.6
1	A	1188	GLN	4.6
2	B	907	GLY	4.6
2	B	404	LYS	4.6
2	B	896	ASP	4.6
1	A	703	THR	4.6
10	J	11	GLY	4.6
1	A	836	TYR	4.6
2	B	30	SER	4.6
1	A	845	LEU	4.6
6	F	140	ASP	4.6
3	C	265	MET	4.6
4	D	174	PRO	4.6
1	A	249	SER	4.6
1	A	577	ILE	4.6
1	A	1312	ASN	4.6
1	A	1367	HIS	4.6
7	G	94	CYS	4.6
2	B	1027	ILE	4.6
9	I	71	SER	4.6
3	C	252	GLN	4.6
1	A	1142	THR	4.6
1	A	1168	GLU	4.6
13	S	183	ASN	4.6
1	A	894	GLU	4.6
2	B	1135	ARG	4.6
1	A	1314	SER	4.6
1	A	1330	ASN	4.6
3	C	83	SER	4.6
7	G	112	LYS	4.6
1	A	627	GLY	4.6

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Mol	Chain	Res	Type	RSRZ
12	L	43	THR	4.6
1	A	63	ARG	4.6
1	A	762	SER	4.6
2	B	309	GLN	4.6
1	A	972	HIS	4.6
8	H	14	GLU	4.6
2	B	130	VAL	4.5
7	G	53	ASN	4.6
2	B	370	PHE	4.5
1	A	706	HIS	4.5
5	E	75	MET	4.5
9	I	67	THR	4.5
2	B	386	LEU	4.5
2	B	844	SER	4.5
3	C	137	LYS	4.5
10	J	49	MET	4.5
1	A	1405	THR	4.5
1	A	691	LEU	4.5
1	A	1268	LEU	4.5
2	B	254	LEU	4.5
1	A	632	VAL	4.5
2	B	824	ILE	4.5
2	B	66	ASP	4.5
1	A	221	SER	4.5
5	E	94	LYS	4.5
1	A	1025	ARG	4.5
3	C	152	GLU	4.5
5	E	157	SER	4.5
1	A	766	GLY	4.5
2	B	913	GLY	4.5
6	F	150	GLU	4.5
2	B	335	GLY	4.5
2	B	116	GLU	4.5
8	H	36	CYS	4.5
2	B	397	ASP	4.5
1	A	1193	LEU	4.5
4	D	128	VAL	4.5
1	A	864	ILE	4.5
2	B	521	LEU	4.5
2	B	993	THR	4.5
1	A	280	GLU	4.5
2	B	696	GLU	4.5

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Mol	Chain	Res	Type	RSRZ
5	E	37	LEU	4.5
8	H	108	SER	4.5
1	A	901	LEU	4.5
5	E	41	ASP	4.5
2	B	901	PRO	4.5
2	B	935	ARG	4.5
2	B	1122	ARG	4.5
5	E	54	GLN	4.5
1	A	269	ILE	4.5
1	A	1187	GLN	4.4
2	B	255	GLN	4.4
1	A	325	ILE	4.4
1	A	311	GLN	4.4
2	B	1040	ASN	4.4
3	C	246	ARG	4.4
3	C	156	THR	4.4
2	B	236	HIS	4.4
2	B	688	GLY	4.4
3	C	196	ASP	4.4
1	A	657	LEU	4.4
1	A	655	PHE	4.4
1	A	307	ASP	4.4
2	B	733	HIS	4.4
2	B	1080	LYS	4.4
1	A	1135	ARG	4.4
8	H	146	ARG	4.4
2	B	37	PHE	4.4
3	C	105	GLY	4.4
1	A	684	ALA	4.4
3	C	14	SER	4.4
2	B	39	ARG	4.4
1	A	13	THR	4.4
1	A	588	LEU	4.4
2	B	108	VAL	4.4
2	B	368	GLU	4.4
1	A	681	GLU	4.4
9	I	46	HIS	4.4
2	B	436	VAL	4.4
2	B	1064	TYR	4.4
1	A	401	GLY	4.4
10	J	55	ASP	4.4
1	A	849	MET	4.3

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Mol	Chain	Res	Type	RSRZ
3	C	120	ILE	4.3
6	F	142	SER	4.3
3	C	146	LYS	4.3
6	F	114	GLU	4.3
1	A	1329	THR	4.3
5	E	154	ILE	4.3
1	A	1265	ASN	4.3
4	D	166	LEU	4.3
2	B	70	ILE	4.3
9	I	63	GLY	4.3
11	K	94	ILE	4.3
2	B	265	SER	4.3
1	A	998	LEU	4.3
7	G	77	VAL	4.3
2	B	1200	ALA	4.3
2	B	366	GLN	4.3
1	A	1011	GLN	4.3
1	A	556	TRP	4.3
2	B	101	MET	4.3
7	G	115	MET	4.3
1	A	636	GLU	4.3
1	A	1222	ASN	4.3
2	B	1044	ALA	4.3
2	B	591	ARG	4.3
1	A	631	HIS	4.3
5	E	130	ALA	4.3
2	B	281	PRO	4.3
2	B	1084	GLN	4.3
13	S	173	HIS	4.3
9	I	14	LEU	4.3
9	I	43	VAL	4.3
8	H	112	ILE	4.3
1	A	152	VAL	4.3
1	A	915	SER	4.3
1	A	570	PRO	4.3
1	A	878	ILE	4.3
2	B	881	ASN	4.2
1	A	964	ILE	4.2
1	A	1175	SER	4.2
1	A	644	LYS	4.2
1	A	1021	LEU	4.2
3	C	136	ASP	4.2

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Mol	Chain	Res	Type	RSRZ
9	I	49	ILE	4.2
1	A	868	TYR	4.2
1	A	271	LYS	4.2
1	A	666	ILE	4.2
2	B	31	TRP	4.2
6	F	85	MET	4.2
13	S	236	LEU	4.2
2	B	1126	GLY	4.2
13	S	151	GLN	4.2
1	A	1133	LEU	4.2
1	A	1443	VAL	4.2
2	B	572	HIS	4.2
1	A	207	ILE	4.2
9	I	21	GLU	4.2
1	A	653	VAL	4.2
3	C	141	GLY	4.2
13	S	300	GLU	4.2
6	F	103	MET	4.2
9	I	77	LYS	4.2
9	I	105	SER	4.2
1	A	858	ASN	4.2
1	A	920	LEU	4.2
5	E	35	VAL	4.2
2	B	377	PHE	4.2
5	E	162	ARG	4.2
5	E	31	THR	4.2
1	A	455	MET	4.2
4	D	146	GLN	4.2
2	B	310	MET	4.2
10	J	31	ASP	4.2
11	K	41	THR	4.2
6	F	120	ILE	4.2
2	B	630	ALA	4.2
1	A	26	GLU	4.2
6	F	83	PRO	4.2
1	A	592	ASP	4.2
11	K	12	LEU	4.1
1	A	422	GLY	4.1
1	A	750	GLY	4.1
1	A	44	THR	4.1
3	C	245	VAL	4.1
2	B	1000	PRO	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	145	LYS	4.1
1	A	186	LYS	4.1
1	A	1094	VAL	4.1
1	A	1004	ASN	4.1
1	A	1009	ASN	4.1
2	B	1095	LEU	4.1
1	A	1352	VAL	4.1
2	B	49	ASP	4.1
2	B	1161	HIS	4.1
1	A	1081	LEU	4.1
13	S	246	GLU	4.1
2	B	865	LYS	4.1
3	C	104	PHE	4.1
9	I	92	ARG	4.1
1	A	718	VAL	4.1
2	B	44	VAL	4.1
1	A	799	PHE	4.1
1	A	263	THR	4.1
2	B	461	LEU	4.1
2	B	1009	ASP	4.1
2	B	770	GLN	4.1
1	A	1134	ILE	4.1
1	A	1445	ILE	4.1
1	A	1404	GLU	4.1
1	A	562	THR	4.1
1	A	900	ASP	4.1
1	A	1308	THR	4.1
1	A	528	LEU	4.1
1	A	1227	ILE	4.1
2	B	903	VAL	4.1
1	A	737	LEU	4.1
1	A	1338	VAL	4.1
1	A	508	PRO	4.1
6	F	99	LEU	4.1
2	B	507	LYS	4.1
2	B	694	ASP	4.1
1	A	1029	ARG	4.1
1	A	598	LEU	4.1
6	F	100	GLN	4.1
2	B	511	PRO	4.1
1	A	1119	TYR	4.1
2	B	848	ARG	4.1

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Mol	Chain	Res	Type	RSRZ
2	B	999	MET	4.1
1	A	543	LEU	4.1
2	B	893	LEU	4.1
3	C	69	LEU	4.1
1	A	389	THR	4.1
1	A	467	THR	4.1
7	G	111	THR	4.1
12	L	60	ARG	4.1
10	J	32	GLU	4.0
2	B	1201	LYS	4.0
1	A	602	ASP	4.0
2	B	680	THR	4.0
7	G	2	PHE	4.0
2	B	1197	PRO	4.0
8	H	24	CYS	4.0
11	K	78	THR	4.0
13	S	242	LYS	4.0
2	B	316	PRO	4.0
3	C	37	MET	4.0
2	B	624	LEU	4.0
1	A	416	ARG	4.0
1	A	693	VAL	4.0
9	I	79	HIS	4.0
1	A	295	LEU	4.0
2	B	523	CYS	4.0
2	B	410	GLY	4.0
1	A	896	ARG	4.0
1	A	1409	LEU	4.0
1	A	135	PHE	4.0
2	B	294	ASP	4.0
2	B	915	THR	4.0
1	A	889	SER	4.0
1	A	1146	VAL	4.0
5	E	212	ARG	4.0
3	C	40	GLU	4.0
1	A	1018	PHE	4.0
2	B	1076	HIS	4.0
1	A	606	LEU	4.0
1	A	956	LEU	4.0
5	E	206	GLY	4.0
1	A	1020	CYS	4.0
1	A	1054	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
2	B	273	LEU	4.0
3	C	151	GLN	4.0
1	A	153	PRO	4.0
2	B	215	GLN	4.0
1	A	486	GLU	4.0
3	C	161	LYS	4.0
8	H	39	THR	4.0
2	B	728	ARG	4.0
1	A	741	ASN	4.0
5	E	201	LYS	4.0
3	C	193	TYR	3.9
1	A	647	GLY	3.9
2	B	381	MET	3.9
3	C	15	LYS	3.9
1	A	1178	ASP	3.9
1	A	1392	SER	3.9
1	A	867	ILE	3.9
2	B	1179	GLN	3.9
1	A	28	ARG	3.9
1	A	800	VAL	3.9
8	H	57	VAL	3.9
2	B	1203	LEU	3.9
7	G	110	VAL	3.9
2	B	348	ARG	3.9
1	A	405	VAL	3.9
6	F	118	LEU	3.9
11	K	97	LYS	3.9
5	E	80	VAL	3.9
2	B	1184	GLY	3.9
2	B	681	TRP	3.9
2	B	872	GLU	3.9
13	S	233	ALA	3.9
2	B	1146	PHE	3.9
9	I	66	PRO	3.9
1	A	619	LYS	3.9
3	C	263	THR	3.9
7	G	95	SER	3.9
6	F	116	ASP	3.9
6	F	134	ILE	3.9
5	E	97	VAL	3.9
1	A	522	GLY	3.9
6	F	111	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	1165	GLU	3.9
3	C	187	LYS	3.9
1	A	127	ALA	3.9
2	B	208	SER	3.9
5	E	77	SER	3.9
1	A	490	HIS	3.9
2	B	1055	ILE	3.8
1	A	11	LEU	3.8
1	A	509	LEU	3.8
1	A	534	LEU	3.8
1	A	1195	LEU	3.8
1	A	365	GLY	3.8
8	H	27	GLU	3.8
2	B	1002	THR	3.8
1	A	169	ASN	3.8
1	A	1089	VAL	3.8
4	D	217	LEU	3.8
6	F	117	PRO	3.8
11	K	77	THR	3.8
1	A	1326	ARG	3.8
2	B	446	LEU	3.8
2	B	535	LEU	3.8
2	B	1028	GLU	3.8
5	E	168	TYR	3.8
1	A	363	GLN	3.8
1	A	242	PRO	3.8
3	C	218	PRO	3.8
2	B	1078	GLY	3.8
3	C	247	GLY	3.8
2	B	104	GLU	3.8
13	S	230	THR	3.8
1	A	1240	CYS	3.8
1	A	561	PRO	3.8
2	B	771	SER	3.8
2	B	560	GLU	3.8
11	K	106	GLU	3.8
1	A	233	TRP	3.8
1	A	301	ALA	3.8
1	A	415	LEU	3.8
1	A	1355	VAL	3.8
2	B	54	PHE	3.8
5	E	61	GLN	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	322	VAL	3.8
1	A	504	LEU	3.8
9	I	98	VAL	3.8
10	J	14	VAL	3.8
2	B	1105	ALA	3.8
13	S	250	LYS	3.7
1	A	1346	ALA	3.7
2	B	767	ASN	3.7
4	D	143	ASN	3.7
1	A	789	LYS	3.7
1	A	711	ARG	3.7
1	A	1174	PHE	3.7
1	A	82	GLY	3.7
1	A	1417	GLU	3.7
1	A	1296	GLY	3.7
13	S	147	LYS	3.7
2	B	784	ASN	3.7
2	B	522	VAL	3.7
2	B	897	GLY	3.7
2	B	32	ALA	3.7
2	B	1140	ALA	3.7
10	J	28	ASP	3.7
2	B	490	SER	3.7
12	L	47	ARG	3.7
5	E	213	ILE	3.7
1	A	682	THR	3.7
2	B	258	LEU	3.7
2	B	741	CYS	3.7
1	A	720	ARG	3.7
1	A	863	VAL	3.7
1	A	548	ASN	3.7
12	L	52	GLY	3.7
1	A	1419	ASP	3.7
2	B	482	VAL	3.7
1	A	531	ILE	3.7
13	S	285	GLN	3.7
2	B	478	GLY	3.7
2	B	544	CYS	3.7
12	L	36	SER	3.7
5	E	193	GLY	3.7
5	E	116	ILE	3.7
1	A	633	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	473	SER	3.7
1	A	1256	GLU	3.7
2	B	853	SER	3.7
1	A	810	PRO	3.7
1	A	872	GLY	3.6
2	B	1173	ALA	3.6
5	E	30	ILE	3.6
5	E	62	ALA	3.6
13	S	212	PRO	3.6
13	S	286	THR	3.6
2	B	55	VAL	3.6
1	A	554	PRO	3.6
4	D	189	ASP	3.6
5	E	44	ALA	3.6
11	K	90	ALA	3.6
13	S	229	ALA	3.6
2	B	263	GLY	3.6
1	A	359	LEU	3.6
5	E	165	LEU	3.6
3	C	157	CYS	3.6
1	A	1328	TYR	3.6
2	B	823	ALA	3.6
2	B	460	ALA	3.6
2	B	1152	MET	3.6
7	G	133	SER	3.6
2	B	550	ASP	3.6
2	B	549	THR	3.6
2	B	553	PRO	3.6
9	I	101	PHE	3.6
1	A	524	VAL	3.6
8	H	114	VAL	3.6
1	A	1440	ALA	3.6
1	A	281	HIS	3.6
1	A	1384	VAL	3.6
1	A	1370	LEU	3.6
2	B	960	GLY	3.6
2	B	858	SER	3.6
2	B	822	ASN	3.6
2	B	908	GLU	3.6
13	S	274	CYS	3.6
1	A	1073	GLY	3.6
2	B	458	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	527	THR	3.5
2	B	1163	CYS	3.5
1	A	743	VAL	3.5
1	A	259	GLU	3.5
6	F	96	THR	3.5
1	A	326	ARG	3.5
1	A	1053	PHE	3.5
2	B	46	GLN	3.5
11	K	17	SER	3.5
11	K	107	THR	3.5
2	B	179	CYS	3.5
1	A	366	VAL	3.5
1	A	1375	MET	3.5
1	A	1389	PHE	3.5
2	B	415	GLN	3.5
2	B	1049	ASP	3.5
1	A	861	GLY	3.5
1	A	1303	GLU	3.5
1	A	1136	SER	3.5
4	D	179	GLN	3.5
1	A	142	CYS	3.5
1	A	855	THR	3.5
4	D	170	THR	3.5
11	K	58	PHE	3.5
2	B	365	THR	3.5
2	B	556	THR	3.5
2	B	755	ILE	3.5
13	S	197	ALA	3.5
1	A	559	VAL	3.5
3	C	234	SER	3.5
1	A	797	LYS	3.5
2	B	810	GLU	3.5
1	A	1299	VAL	3.5
3	C	48	SER	3.5
8	H	105	GLU	3.5
1	A	968	GLN	3.5
1	A	825	ILE	3.5
2	B	495	LEU	3.5
2	B	686	ASN	3.5
2	B	1025	HIS	3.5
8	H	43	ASN	3.5
13	S	270	THR	3.5

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Mol	Chain	Res	Type	RSRZ
5	E	147	HIS	3.5
1	A	1180	GLU	3.5
1	A	332	LYS	3.5
5	E	205	SER	3.5
1	A	630	ILE	3.5
1	A	988	LEU	3.5
2	B	599	THR	3.5
11	K	83	PRO	3.5
2	B	360	PHE	3.5
1	A	1037	LEU	3.4
3	C	129	ILE	3.4
11	K	6	ARG	3.4
1	A	994	GLN	3.4
1	A	65	LEU	3.4
1	A	1416	ALA	3.4
1	A	926	GLN	3.4
1	A	414	ASP	3.4
1	A	489	LEU	3.4
10	J	9	SER	3.4
1	A	81	PHE	3.4
1	A	492	PRO	3.4
2	B	1117	GLN	3.4
3	C	221	TYR	3.4
1	A	884	ASP	3.4
1	A	1137	ALA	3.4
1	A	1282	VAL	3.4
2	B	609	ILE	3.4
8	H	103	LYS	3.4
2	B	818	PRO	3.4
3	C	251	LEU	3.4
10	J	18	TRP	3.4
2	B	494	HIS	3.4
1	A	553	VAL	3.4
2	B	261	ARG	3.4
1	A	361	LEU	3.4
2	B	1128	LEU	3.4
1	A	154	SER	3.4
11	K	16	GLU	3.4
2	B	528	PRO	3.4
1	A	223	GLY	3.4
1	A	341	MET	3.4
3	C	107	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	1183	GLN	3.4
3	C	195	GLN	3.4
1	A	757	ASN	3.4
2	B	388	CYS	3.4
2	B	974	PRO	3.4
1	A	776	ALA	3.4
1	A	352	VAL	3.4
1	A	1446	ASP	3.4
1	A	1044	TRP	3.4
2	B	797	TYR	3.4
1	A	966	ASN	3.4
2	B	794	ASN	3.4
2	B	220	GLY	3.4
5	E	141	VAL	3.4
1	A	46	THR	3.3
1	A	1294	PRO	3.3
2	B	795	ILE	3.3
7	G	67	SER	3.3
2	B	584	GLY	3.3
5	E	150	VAL	3.3
8	H	16	ASP	3.3
11	K	99	GLY	3.3
2	B	1079	LYS	3.3
2	B	195	CYS	3.3
11	K	111	LEU	3.3
2	B	834	ASN	3.3
9	I	15	TYR	3.3
8	H	104	PHE	3.3
2	B	227	LYS	3.3
4	D	139	LYS	3.3
2	B	205	ILE	3.3
1	A	305	ASP	3.3
1	A	759	ALA	3.3
2	B	34	ILE	3.3
1	A	770	VAL	3.3
11	K	65	HIS	3.3
1	A	25	GLU	3.3
2	B	186	GLU	3.3
13	S	302	CYS	3.3
2	B	40	GLU	3.3
6	F	132	LEU	3.3
1	A	1369	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	433	GLU	3.3
2	B	426	LYS	3.3
6	F	86	THR	3.3
1	A	699	ALA	3.3
2	B	1144	ALA	3.3
1	A	79	GLY	3.3
3	C	98	VAL	3.3
7	G	137	ILE	3.3
1	A	39	GLU	3.3
2	B	1004	GLU	3.3
1	A	461	LYS	3.3
1	A	840	ARG	3.3
3	C	116	LYS	3.3
1	A	1332	PHE	3.3
8	H	143	LEU	3.3
1	A	899	VAL	3.3
2	B	355	ILE	3.3
3	C	103	ALA	3.3
1	A	247	ARG	3.3
2	B	636	PRO	3.3
2	B	981	ALA	3.3
3	C	85	ASP	3.3
3	C	32	SER	3.3
2	B	957	ASN	3.2
10	J	35	ALA	3.2
4	D	145	MET	3.2
1	A	1091	SER	3.2
1	A	954	TRP	3.2
2	B	664	THR	3.2
5	E	90	VAL	3.2
1	A	925	LEU	3.2
2	B	508	LEU	3.2
1	A	240	PRO	3.2
3	C	106	GLU	3.2
6	F	148	VAL	3.2
2	B	956	THR	3.2
10	J	21	TYR	3.2
8	H	137	GLN	3.2
1	A	1023	ARG	3.2
11	K	27	ALA	3.2
3	C	177	GLU	3.2
8	H	145	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	642	CYS	3.2
1	A	1016	THR	3.2
2	B	603	LEU	3.2
7	G	109	PHE	3.2
1	A	375	THR	3.2
2	B	776	GLN	3.2
4	D	157	GLN	3.2
1	A	1379	GLY	3.2
2	B	714	GLU	3.2
1	A	1159	ARG	3.2
5	E	127	ILE	3.2
2	B	1218	THR	3.2
4	D	187	THR	3.2
3	C	61	GLU	3.2
5	E	21	GLU	3.2
11	K	1	MET	3.2
2	B	643	ASP	3.2
1	A	107	CYS	3.2
3	C	231	ASN	3.2
13	S	255	ASN	3.2
11	K	31	VAL	3.2
1	A	1152	ILE	3.2
1	A	355	GLY	3.2
1	A	265	LYS	3.2
1	A	462	VAL	3.2
8	H	92	ASP	3.2
1	A	119	ASN	3.2
1	A	824	LEU	3.2
2	B	852	ARG	3.2
1	A	402	ALA	3.1
1	A	1049	ILE	3.1
3	C	145	CYS	3.1
13	S	150	ASP	3.1
3	C	138	GLU	3.1
5	E	58	MET	3.1
3	C	7	GLN	3.1
13	S	165	GLU	3.1
2	B	1188	LYS	3.1
1	A	387	ARG	3.1
1	A	1279	ILE	3.1
1	A	857	ARG	3.1
1	A	610	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
5	E	202	SER	3.1
2	B	110	HIS	3.1
13	S	223	ILE	3.1
13	S	293	LEU	3.1
2	B	403	LYS	3.1
1	A	668	ASP	3.1
1	A	100	LYS	3.1
1	A	934	LYS	3.1
2	B	375	ALA	3.1
2	B	769	TYR	3.1
2	B	463	THR	3.1
11	K	24	ASP	3.1
1	A	942	PHE	3.1
1	A	1438	THR	3.1
10	J	23	ASN	3.1
2	B	846	ILE	3.1
1	A	950	GLY	3.1
2	B	1096	ARG	3.1
1	A	34	LYS	3.1
3	C	9	LYS	3.1
1	A	50	ILE	3.1
1	A	848	ILE	3.1
2	B	563	MET	3.1
2	B	492	LEU	3.1
11	K	88	LYS	3.1
1	A	983	ILE	3.1
2	B	871	THR	3.1
1	A	1185	PHE	3.1
2	B	1005	GLY	3.1
2	B	1043	ASP	3.1
1	A	441	PRO	3.1
1	A	1147	THR	3.1
5	E	169	ARG	3.1
2	B	1141	HIS	3.1
5	E	164	LEU	3.1
1	A	1198	ASP	3.1
2	B	225	VAL	3.1
2	B	447	ALA	3.1
2	B	817	LEU	3.1
5	E	65	THR	3.1
1	A	1274	ARG	3.0
2	B	766	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	904	ARG	3.0
1	A	111	GLY	3.0
1	A	539	THR	3.0
1	A	1313	LEU	3.0
2	B	945	GLU	3.0
10	J	48	ARG	3.0
1	A	410	GLY	3.0
1	A	1078	GLN	3.0
2	B	936	ASP	3.0
1	A	613	ILE	3.0
2	B	1071	VAL	3.0
11	K	34	THR	3.0
11	K	44	ASN	3.0
1	A	1395	GLY	3.0
1	A	59	GLY	3.0
2	B	826	ALA	3.0
11	K	20	LYS	3.0
2	B	214	ALA	3.0
8	H	61	SER	3.0
5	E	176	PRO	3.0
7	G	83	LYS	3.0
8	H	9	ILE	3.0
3	C	183	TRP	3.0
8	H	82	PRO	3.0
1	A	1063	MET	3.0
9	I	84	VAL	3.0
5	E	118	PRO	3.0
4	D	135	GLY	3.0
13	S	194	ALA	3.0
1	A	961	ARG	3.0
1	A	1100	ARG	3.0
7	G	21	ARG	3.0
1	A	535	THR	3.0
1	A	596	THR	3.0
1	A	746	MET	3.0
2	B	809	MET	3.0
2	B	821	GLN	3.0
3	C	158	VAL	3.0
3	C	99	LEU	3.0
1	A	856	THR	3.0
2	B	1115	THR	3.0
1	A	432	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	584	ASN	3.0
3	C	162	GLY	3.0
7	G	66	GLY	3.0
8	H	99	GLY	3.0
3	C	119	VAL	3.0
5	E	121	MET	3.0
1	A	89	PRO	3.0
2	B	1143	ALA	3.0
7	G	72	VAL	3.0
2	B	21	GLU	3.0
1	A	202	LEU	3.0
1	A	740	LEU	3.0
2	B	259	TYR	3.0
3	C	28	ALA	3.0
3	C	79	GLN	3.0
2	B	319	GLU	2.9
2	B	600	LEU	2.9
9	I	24	ARG	2.9
2	B	1001	PHE	2.9
1	A	246	VAL	2.9
1	A	898	ARG	2.9
3	C	149	LYS	2.9
7	G	44	TYR	2.9
2	B	1075	GLY	2.9
2	B	1033	LYS	2.9
1	A	1214	GLU	2.9
1	A	1191	TRP	2.9
1	A	841	LEU	2.9
8	H	139	ASN	2.9
1	A	1204	ASP	2.9
2	B	376	PHE	2.9
13	S	239	ALA	2.9
1	A	471	ASN	2.9
3	C	188	HIS	2.9
9	I	35	VAL	2.9
3	C	122	SER	2.9
2	B	1011	ILE	2.9
13	S	259	ALA	2.9
3	C	76	ASP	2.9
3	C	96	SER	2.9
12	L	69	ALA	2.9
5	E	134	THR	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
8	H	128	ASN	2.9
1	A	520	CYS	2.9
2	B	620	ARG	2.9
2	B	1215	ARG	2.9
3	C	24	ASN	2.9
1	A	133	LYS	2.9
8	H	42	ILE	2.9
2	B	1208	MET	2.9
5	E	46	TYR	2.9
1	A	604	GLY	2.9
1	A	688	LYS	2.9
1	A	1226	VAL	2.9
7	G	107	LYS	2.9
13	S	240	PRO	2.9
1	A	811	GLN	2.9
1	A	1273	LEU	2.9
2	B	610	ASN	2.9
2	B	748	ILE	2.9
3	C	267	GLN	2.9
1	A	147	VAL	2.8
3	C	254	LYS	2.8
2	B	1018	PRO	2.8
3	C	213	PRO	2.8
1	A	752	LYS	2.8
3	C	13	ALA	2.8
2	B	384	ARG	2.8
1	A	928	LEU	2.8
2	B	1113	VAL	2.8
6	F	80	ALA	2.8
1	A	870	GLU	2.8
2	B	1074	ASN	2.8
1	A	391	LEU	2.8
1	A	621	THR	2.8
1	A	676	MET	2.8
4	D	117	GLU	2.8
1	A	893	PHE	2.8
5	E	188	LEU	2.8
1	A	761	MET	2.8
2	B	385	LEU	2.8
4	D	208	GLU	2.8
5	E	95	THR	2.8
1	A	782	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	500	GLU	2.8
2	B	909	ASP	2.8
4	D	123	LEU	2.8
1	A	1278	ASN	2.8
1	A	1045	VAL	2.8
1	A	662	PHE	2.8
2	B	526	GLU	2.8
13	S	275	LYS	2.8
2	B	1060	ARG	2.8
2	B	1219	ASP	2.8
2	B	454	THR	2.8
7	G	169	GLY	2.8
1	A	624	SER	2.8
2	B	1165	ILE	2.8
1	A	652	VAL	2.8
1	A	1372	VAL	2.8
1	A	620	LYS	2.8
2	B	352	ALA	2.8
1	A	350	ARG	2.8
2	B	841	MET	2.8
1	A	1003	LYS	2.8
1	A	1051	ALA	2.8
6	F	125	LEU	2.8
1	A	1447	GLU	2.8
2	B	1213	THR	2.8
1	A	725	ALA	2.8
1	A	1423	GLY	2.8
2	B	91	SER	2.8
5	E	108	GLY	2.8
2	B	958	GLN	2.8
1	A	451	HIS	2.7
2	B	372	SER	2.7
2	B	480	SER	2.7
3	C	126	GLY	2.8
1	A	846	GLU	2.7
2	B	1094	ARG	2.7
2	B	326	ASP	2.7
2	B	978	ASP	2.7
1	A	844	ALA	2.7
1	A	1032	LEU	2.7
1	A	505	CYS	2.7
2	B	602	THR	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
10	J	60	PHE	2.7
11	K	60	ALA	2.7
1	A	747	VAL	2.7
2	B	1171	VAL	2.7
2	B	994	TYR	2.7
1	A	139	TRP	2.7
6	F	145	ASP	2.7
3	C	100	THR	2.7
2	B	363	HIS	2.7
7	G	168	LEU	2.7
1	A	300	VAL	2.7
5	E	26	ARG	2.7
1	A	922	ASP	2.7
11	K	62	LYS	2.7
1	A	225	ASN	2.7
2	B	176	SER	2.7
1	A	1300	LYS	2.7
2	B	50	SER	2.7
3	C	153	LEU	2.7
6	F	138	LEU	2.7
3	C	54	ASN	2.7
5	E	136	ASN	2.7
3	C	181	ASP	2.7
1	A	754	SER	2.7
2	B	788	ARG	2.7
5	E	142	VAL	2.7
11	K	48	ALA	2.7
1	A	1209	MET	2.7
1	A	1411	GLU	2.7
2	B	113	TYR	2.7
2	B	772	ALA	2.7
3	C	36	VAL	2.7
5	E	183	PRO	2.7
8	H	12	VAL	2.7
3	C	128	ASN	2.7
1	A	303	TYR	2.7
2	B	1016	ALA	2.7
2	B	1172	ILE	2.7
1	A	590	ARG	2.7
2	B	965	LYS	2.7
1	A	429	GLY	2.7
2	B	950	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
3	C	55	THR	2.7
1	A	364	VAL	2.7
1	A	267	ALA	2.7
13	S	188	CYS	2.7
5	E	111	VAL	2.7
1	A	371	ALA	2.7
1	A	772	GLY	2.7
1	A	1008	GLN	2.7
2	B	479	VAL	2.7
1	A	357	PRO	2.7
2	B	1008	PRO	2.7
7	G	15	PRO	2.7
1	A	517	ASN	2.7
6	F	87	LYS	2.7
1	A	571	LEU	2.6
3	C	71	PRO	2.6
1	A	1024	SER	2.6
1	A	204	THR	2.6
1	A	1086	PHE	2.6
13	S	181	GLU	2.6
2	B	1021	MET	2.6
2	B	234	ILE	2.6
2	B	1167	GLY	2.6
7	G	68	ALA	2.6
2	B	685	LEU	2.6
9	I	6	PHE	2.6
3	C	35	ARG	2.6
3	C	175	ALA	2.6
5	E	181	ALA	2.6
8	H	63	LEU	2.6
5	E	33	GLU	2.6
5	E	160	GLU	2.6
1	A	385	ILE	2.6
1	A	296	LEU	2.6
3	C	111	THR	2.6
1	A	1092	LYS	2.6
5	E	57	MET	2.6
1	A	97	ALA	2.6
4	D	132	GLN	2.6
11	K	38	GLU	2.6
1	A	875	ALA	2.6
2	B	1037	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	32	VAL	2.6
1	A	921	GLY	2.6
1	A	293	GLU	2.6
2	B	182	SER	2.6
2	B	1150	ARG	2.6
11	K	61	TYR	2.6
1	A	299	HIS	2.6
1	A	980	ASP	2.6
1	A	802	ASN	2.6
13	S	211	ASN	2.6
5	E	137	GLU	2.6
2	B	264	SER	2.6
10	J	29	GLU	2.6
1	A	719	VAL	2.6
12	L	45	ALA	2.6
2	B	303	TYR	2.6
2	B	805	THR	2.6
5	E	175	LEU	2.6
2	B	243	ALA	2.6
1	A	122	MET	2.6
1	A	488	ASN	2.5
2	B	48	LEU	2.5
2	B	545	ILE	2.5
7	G	157	ILE	2.5
1	A	1285	MET	2.5
3	C	19	ASP	2.5
1	A	516	SER	2.5
2	B	959	ASP	2.5
1	A	532	ARG	2.5
2	B	506	GLY	2.5
1	A	1415	SER	2.5
2	B	982	SER	2.5
2	B	407	ASP	2.5
6	F	81	THR	2.5
2	B	1072	MET	2.5
2	B	115	GLN	2.5
13	S	288	SER	2.5
1	A	368	LYS	2.5
7	G	159	ALA	2.5
1	A	14	VAL	2.5
3	C	18	VAL	2.5
2	B	185	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	1047	SER	2.5
1	A	1125	ALA	2.5
8	H	133	ASN	2.5
1	A	372	LYS	2.5
2	B	558	LEU	2.5
1	A	131	SER	2.5
2	B	63	ILE	2.5
2	B	361	LEU	2.5
2	B	1024	ALA	2.5
5	E	64	PRO	2.5
2	B	1148	LYS	2.5
1	A	177	ASP	2.5
2	B	726	ALA	2.5
3	C	64	ALA	2.5
7	G	84	GLY	2.5
1	A	552	TRP	2.5
1	A	990	VAL	2.5
2	B	33	VAL	2.5
2	B	378	LEU	2.5
2	B	287	ARG	2.5
7	G	163	ILE	2.5
2	B	543	SER	2.5
4	D	206	GLU	2.5
5	E	98	ILE	2.5
2	B	877	PRO	2.5
2	B	1051	THR	2.5
1	A	550	LEU	2.5
2	B	976	ILE	2.5
3	C	27	LEU	2.5
1	A	586	ILE	2.5
1	A	679	ILE	2.5
1	A	952	ALA	2.5
2	B	995	ARG	2.5
11	K	100	ALA	2.5
1	A	329	LEU	2.4
2	B	498	THR	2.4
1	A	230	ARG	2.4
1	A	507	VAL	2.4
1	A	751	SER	2.4
1	A	1238	ILE	2.4
2	B	477	ALA	2.4
1	A	614	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	1340	GLY	2.4
1	A	593	GLU	2.4
2	B	244	LEU	2.4
6	F	137	TYR	2.4
2	B	839	MET	2.4
11	K	72	LYS	2.4
2	B	1090	THR	2.4
2	B	1010	LEU	2.4
2	B	596	LEU	2.4
2	B	238	ALA	2.4
2	B	551	PRO	2.4
2	B	1088	GLY	2.4
12	L	59	ALA	2.4
1	A	466	SER	2.4
1	A	902	LEU	2.4
2	B	41	LYS	2.4
2	B	687	GLU	2.4
2	B	1119	VAL	2.4
5	E	20	LYS	2.4
3	C	248	ILE	2.4
5	E	178	ILE	2.4
1	A	66	LYS	2.4
2	B	813	LYS	2.4
11	K	70	ARG	2.4
13	S	200	ARG	2.4
13	S	264	SER	2.4
1	A	232	GLU	2.4
1	A	384	ASN	2.4
1	A	712	GLU	2.4
2	B	1068	GLY	2.4
7	G	79	PHE	2.4
10	J	1	MET	2.4
2	B	513	GLN	2.4
11	K	57	LEU	2.4
13	S	305	ARG	2.4
1	A	638	GLY	2.4
13	S	304	ASN	2.4
1	A	21	LEU	2.4
1	A	498	ARG	2.4
1	A	1345	ARG	2.4
1	A	963	ILE	2.4
1	A	1360	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	1027	ALA	2.4
1	A	17	VAL	2.4
1	A	1206	ASP	2.4
8	H	10	PHE	2.4
1	A	648	ASN	2.4
2	B	483	LEU	2.4
2	B	883	LEU	2.4
4	D	129	LEU	2.4
6	F	155	LEU	2.4
9	I	11	ASN	2.4
1	A	851	HIS	2.4
2	B	706	GLN	2.4
2	B	997	GLU	2.4
12	L	68	GLU	2.4
1	A	165	GLY	2.4
1	A	700	ASN	2.4
1	A	812	GLU	2.4
1	A	1365	TYR	2.4
2	B	1194	ILE	2.4
13	S	184	LYS	2.4
1	A	547	LEU	2.4
2	B	119	LEU	2.4
13	S	190	THR	2.4
1	A	427	GLN	2.4
1	A	587	HIS	2.4
1	A	763	ALA	2.4
7	G	92	VAL	2.4
2	B	1006	ILE	2.3
4	D	151	PHE	2.4
1	A	1033	GLN	2.3
7	G	69	GLU	2.3
2	B	400	HIS	2.3
1	A	98	LYS	2.3
2	B	764	SER	2.3
2	B	838	SER	2.3
1	A	143	LYS	2.3
2	B	536	VAL	2.3
3	C	173	ALA	2.3
1	A	83	HIS	2.3
1	A	84	ILE	2.3
11	K	47	ARG	2.3
8	H	123	MET	2.3

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Mol	Chain	Res	Type	RSRZ
13	S	232	ASP	2.3
10	J	59	LYS	2.3
1	A	454	SER	2.3
1	A	734	GLU	2.3
2	B	644	GLU	2.3
3	C	233	GLU	2.3
2	B	1158	PHE	2.3
1	A	523	ILE	2.3
2	B	827	ILE	2.3
3	C	179	GLU	2.3
7	G	122	ASN	2.3
1	A	1259	MET	2.3
2	B	260	GLY	2.3
5	E	107	THR	2.3
2	B	825	VAL	2.3
7	G	5	LYS	2.3
6	F	91	ALA	2.3
8	H	21	ASN	2.3
1	A	1190	PRO	2.3
1	A	217	LYS	2.3
2	B	541	LEU	2.3
2	B	612	GLU	2.3
2	B	697	GLU	2.3
2	B	979	LYS	2.3
1	A	137	ALA	2.3
2	B	874	PHE	2.3
1	A	769	SER	2.3
4	D	209	ARG	2.3
1	A	1170	ILE	2.3
2	B	964	VAL	2.3
7	G	90	THR	2.3
1	A	469	ARG	2.3
1	A	686	ALA	2.3
6	F	101	ILE	2.3
3	C	154	LYS	2.3
5	E	25	ASP	2.3
2	B	589	VAL	2.3
13	S	215	LYS	2.3
2	B	691	GLU	2.3
1	A	635	ARG	2.3
3	C	87	PHE	2.3
1	A	304	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	1284	MET	2.3
2	B	111	ALA	2.3
5	E	117	THR	2.3
2	B	1192	TYR	2.3
1	A	342	GLY	2.3
2	B	423	LYS	2.3
2	B	762	ASN	2.3
2	B	459	TYR	2.3
12	L	29	TYR	2.3
1	A	443	LEU	2.2
1	A	982	THR	2.2
1	A	911	SER	2.2
1	A	208	LEU	2.2
1	A	651	LYS	2.2
1	A	599	SER	2.2
1	A	47	ARG	2.2
1	A	237	THR	2.2
1	A	544	ASP	2.2
2	B	876	LYS	2.2
3	C	169	LYS	2.2
4	D	205	ASP	2.2
13	S	278	LYS	2.2
1	A	661	GLY	2.2
4	D	121	LYS	2.2
13	S	247	GLU	2.2
1	A	888	GLY	2.2
1	A	1335	ILE	2.2
2	B	750	GLY	2.2
1	A	639	PRO	2.2
1	A	1096	SER	2.2
2	B	242	SER	2.2
4	D	175	PHE	2.2
13	S	227	PHE	2.2
1	A	1318	THR	2.2
1	A	1398	MET	2.2
2	B	850	LEU	2.2
2	B	307	ASP	2.2
2	B	1093	GLN	2.2
1	A	764	CYS	2.2
5	E	9	ILE	2.2
1	A	56	PRO	2.2
2	B	829	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	818	MET	2.2
7	G	131	GLN	2.2
11	K	104	ASN	2.2
13	S	235	ASP	2.2
1	A	354	SER	2.2
1	A	929	LEU	2.2
1	A	1297	GLU	2.2
3	C	260	LEU	2.2
1	A	813	PHE	2.2
2	B	777	ALA	2.2
2	B	842	ASN	2.2
2	B	1196	ILE	2.2
3	C	147	LEU	2.2
1	A	339	ASN	2.2
2	B	765	PRO	2.2
8	H	26	ILE	2.2
3	C	178	PHE	2.2
5	E	47	CYS	2.2
1	A	1164	PRO	2.2
1	A	1097	GLY	2.2
1	A	1194	ARG	2.2
1	A	1266	THR	2.2
5	E	207	ARG	2.2
2	B	1003	ALA	2.2
2	B	1059	LEU	2.2
5	E	186	LEU	2.2
9	I	20	LYS	2.2
11	K	32	VAL	2.2
1	A	869	GLY	2.2
10	J	34	THR	2.2
13	S	174	THR	2.2
1	A	546	VAL	2.2
2	B	695	ALA	2.2
7	G	162	SER	2.2
13	S	213	ASP	2.2
3	C	81	GLU	2.2
5	E	102	GLU	2.2
1	A	536	LEU	2.1
1	A	1071	SER	2.1
4	D	138	ASN	2.1
5	E	70	SER	2.1
13	S	195	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
13	S	210	ASN	2.1
1	A	19	PHE	2.1
1	A	943	LEU	2.1
9	I	25	LEU	2.1
1	A	18	GLN	2.1
2	B	757	PRO	2.1
1	A	907	THR	2.1
2	B	53	GLN	2.1
2	B	94	LYS	2.1
2	B	512	ARG	2.1
1	A	612	ILE	2.1
1	A	814	PHE	2.1
1	A	819	GLY	2.1
6	F	141	GLY	2.1
8	H	30	SER	2.1
11	K	108	GLU	2.1
13	S	306	TRP	2.1
2	B	194	GLU	2.1
1	A	512	VAL	2.1
1	A	521	MET	2.1
1	A	1177	LEU	2.1
2	B	629	ASP	2.1
2	B	231	PRO	2.1
11	K	75	ILE	2.1
2	B	641	GLU	2.1
11	K	18	LYS	2.1
1	A	1080	THR	2.1
2	B	1176	ASN	2.1
9	I	16	PRO	2.1
2	B	947	GLY	2.1
2	B	1164	GLY	2.1
4	D	192	LYS	2.1
3	C	11	ARG	2.1
2	B	659	ALA	2.1
2	B	828	ALA	2.1
10	J	54	VAL	2.1
1	A	1354	ASN	2.1
2	B	991	GLY	2.1
10	J	47	ARG	2.1
1	A	376	TYR	2.1
2	B	906	SER	2.1
9	I	108	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	78	PRO	2.1
2	B	408	LEU	2.1
2	B	532	ALA	2.1
7	G	17	PHE	2.1
4	D	155	ARG	2.1
1	A	456	MET	2.1
2	B	191	LYS	2.1
1	A	93	VAL	2.1
1	A	327	ALA	2.1
1	A	1270	ASN	2.1
2	B	833	TYR	2.1
3	C	226	ASP	2.1
3	C	239	PRO	2.1
4	D	169	SER	2.1
2	B	500	THR	2.1
2	B	1222	ARG	2.1
1	A	292	ALA	2.0
4	D	221	TYR	2.0
1	A	236	LEU	2.0
1	A	180	LYS	2.0
1	A	566	ILE	2.0
1	A	87	ALA	2.0
11	K	23	PRO	2.0
12	L	67	PHE	2.0
1	A	1380	GLY	2.0
1	A	607	ILE	2.0
1	A	1201	ALA	2.0
2	B	1083	ALA	2.0
1	A	947	PHE	2.0
8	H	127	GLY	2.0
2	B	172	ILE	2.0
8	H	144	ILE	2.0
1	A	579	SER	2.0
3	C	39	ALA	2.0
4	D	188	ALA	2.0
1	A	377	PRO	2.0
1	A	575	LYS	2.0
1	A	1107	VAL	2.0
3	C	220	ASP	2.0
8	H	94	ASP	2.0
1	A	991	LYS	2.0
8	H	97	MET	2.0

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Mol	Chain	Res	Type	RSRZ
9	I	85	PHE	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
15	ZN	J	100	1/1	0.98	0.20	-	30,30,30,30	0
15	ZN	C	319	1/1	0.98	0.20	-	30,30,30,30	0
15	ZN	A	1736	1/1	0.97	0.20	-	30,30,30,30	0
15	ZN	B	1300	1/1	0.97	0.23	-	30,30,30,30	0
15	ZN	S	400	1/1	0.94	0.18	-	30,30,30,30	0
15	ZN	I	201	1/1	0.96	0.15	-	30,30,30,30	0
15	ZN	I	200	1/1	0.98	0.22	-	30,30,30,30	0
15	ZN	A	1735	1/1	0.95	0.18	-	30,30,30,30	0
14	MG	A	1734	1/1	0.63	0.24	-	61,61,61,61	0
15	ZN	L	100	1/1	0.96	0.13	-	30,30,30,30	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.