



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 11:43 PM GMT

PDB ID : 5CBM  
Title : Crystal structure of PfA-M17 with virtual ligand inhibitor  
Authors : Ruggeri, C.; Drinkwater, N.; McGowan, S.  
Deposited on : 2015-07-01  
Resolution : 2.30 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  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20026982

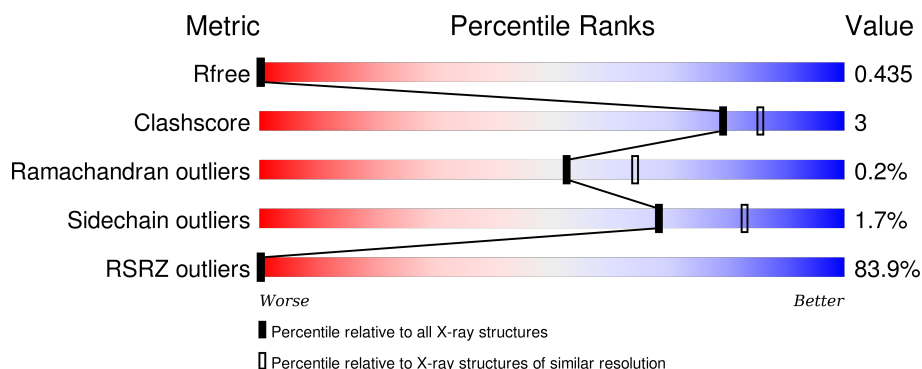
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	519	<div> <div>87%</div> <div> <div>92%</div> <div>8%</div> </div> </div>
1	B	519	<div> <div>84%</div> <div> <div>89%</div> <div>10%</div> <div>.</div> </div> </div>
1	C	519	<div> <div>87%</div> <div> <div>91%</div> <div>9%</div> </div> </div>
1	D	519	<div> <div>77%</div> <div> <div>89%</div> <div>10%</div> <div>.</div> </div> </div>
1	E	519	<div> <div>82%</div> <div> <div>90%</div> <div>8%</div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	519	<div> <div>82%</div> <div>90%</div> <div>8%</div> </div>
1	G	519	<div> <div>86%</div> <div>90%</div> <div>10%</div> </div>
1	H	519	<div> <div>86%</div> <div>90%</div> <div>9%</div> </div>
1	I	519	<div> <div>84%</div> <div>92%</div> <div>7%</div> </div>
1	J	519	<div> <div>79%</div> <div>87%</div> <div>11%</div> </div>
1	K	519	<div> <div>82%</div> <div>92%</div> <div>6%</div> </div>
1	L	519	<div> <div>82%</div> <div>90%</div> <div>8%</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CO3	D	701	-	-	-	X
2	CO3	E	701	-	-	-	X
2	CO3	J	701	-	-	-	X
2	CO3	K	701	-	-	-	X
4	4ZN	B	704	-	-	-	X
4	4ZN	D	704	-	-	-	X
4	4ZN	E	704	-	-	-	X
4	4ZN	F	704	-	-	-	X
4	4ZN	G	704	-	-	-	X
4	4ZN	H	704	-	-	-	X
4	4ZN	L	704	-	-	-	X
5	1PE	A	705	-	-	-	X
5	1PE	B	705	-	-	-	X
5	1PE	D	706	-	-	-	X
5	1PE	G	705	-	-	-	X
5	1PE	G	706	-	-	-	X
5	1PE	G	707	-	-	-	X
5	1PE	H	706	-	-	-	X
5	1PE	I	706	-	-	-	X
5	1PE	J	705	-	-	-	X
5	1PE	J	707	-	-	-	X
5	1PE	K	706	-	-	-	X
5	1PE	L	705	-	-	-	X
7	SO4	A	708	-	-	-	X
7	SO4	A	711	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	SO4	A	712	-	-	X	X
7	SO4	C	708	-	-	-	X
7	SO4	C	710	-	-	-	X
7	SO4	C	711	-	-	-	X
7	SO4	E	709	-	-	-	X
7	SO4	F	707	-	-	-	X
7	SO4	G	711	-	-	X	X
7	SO4	K	708	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 50850 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 M17 family aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	519	Total	C	N	O	S	0	1	0
			3971	2547	639	766	19			
1	B	516	Total	C	N	O	S	0	0	0
			3902	2509	633	740	20			
1	C	517	Total	C	N	O	S	0	0	0
			3941	2532	637	753	19			
1	D	514	Total	C	N	O	S	0	0	0
			3920	2526	633	741	20			
1	E	509	Total	C	N	O	S	0	0	0
			3893	2509	624	741	19			
1	F	511	Total	C	N	O	S	0	0	0
			3851	2477	622	733	19			
1	G	519	Total	C	N	O	S	0	0	0
			3974	2554	640	760	20			
1	H	517	Total	C	N	O	S	1	0	0
			3902	2508	632	743	19			
1	I	517	Total	C	N	O	S	0	0	0
			3951	2540	637	754	20			
1	J	514	Total	C	N	O	S	0	0	0
			3926	2529	633	744	20			
1	K	509	Total	C	N	O	S	0	0	0
			3884	2504	623	738	19			
1	L	511	Total	C	N	O	S	0	0	0
			3848	2475	622	732	19			

There are 36 discrepancies between the modelled and reference sequences:

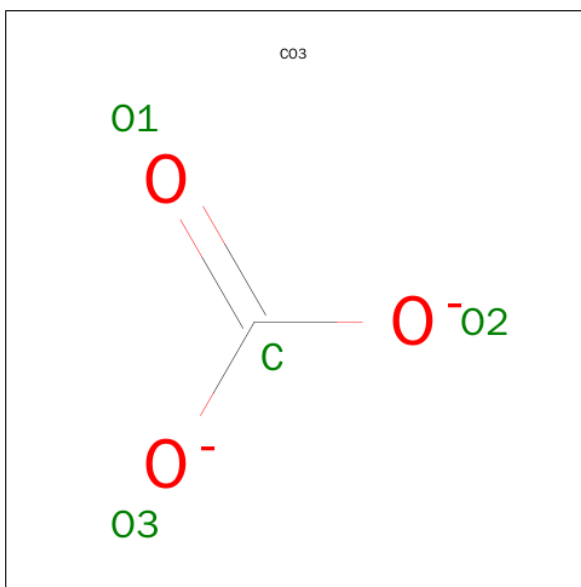
Chain	Residue	Modelled	Actual	Comment	Reference
A	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
A	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
A	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
B	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
B	515	GLN	ASN	engineered mutation	UNP A0A024V0B1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
C	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
C	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
C	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
D	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
D	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
D	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
E	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
E	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
E	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
F	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
F	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
F	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
G	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
G	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
G	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
H	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
H	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
H	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
I	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
I	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
I	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
J	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
J	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
J	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
K	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
K	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
K	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
L	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
L	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
L	546	GLN	ASN	engineered mutation	UNP A0A024V0B1

- Molecule 2 is CARBONATE ION (three-letter code: CO3) (formula: CO<sub>3</sub>).

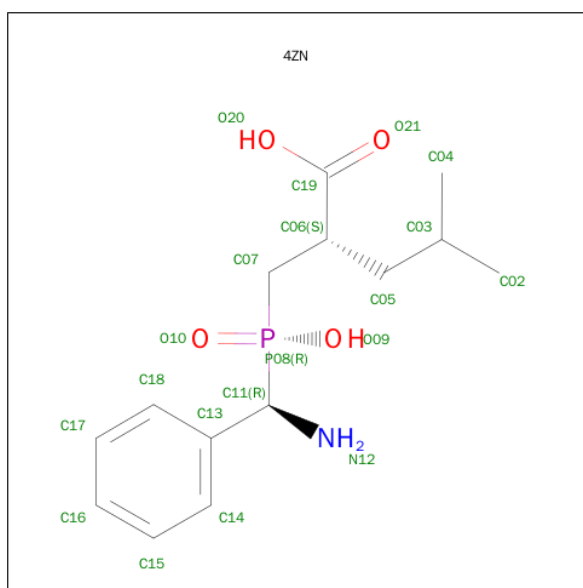


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	1	3		
2	B	1	Total	C	O	0	0
			4	1	3		
2	C	1	Total	C	O	0	0
			4	1	3		
2	D	1	Total	C	O	0	0
			4	1	3		
2	E	1	Total	C	O	0	0
			4	1	3		
2	F	1	Total	C	O	0	0
			4	1	3		
2	G	1	Total	C	O	0	0
			4	1	3		
2	H	1	Total	C	O	0	0
			4	1	3		
2	I	1	Total	C	O	0	0
			4	1	3		
2	J	1	Total	C	O	0	0
			4	1	3		
2	K	1	Total	C	O	0	0
			4	1	3		
2	L	1	Total	C	O	0	0
			4	1	3		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	2	Total 2    Zn 2    2	0	0
3	J	2	Total 2    Zn 2    2	0	0
3	D	2	Total 2    Zn 2    2	0	0
3	K	2	Total 2    Zn 2    2	0	0
3	E	2	Total 2    Zn 2    2	0	0
3	H	2	Total 2    Zn 2    2	0	0
3	B	2	Total 2    Zn 2    2	0	0
3	I	2	Total 2    Zn 2    2	0	0
3	C	2	Total 2    Zn 2    2	0	0
3	A	2	Total 2    Zn 2    2	0	0
3	L	2	Total 2    Zn 2    2	0	0
3	F	2	Total 2    Zn 2    2	0	0

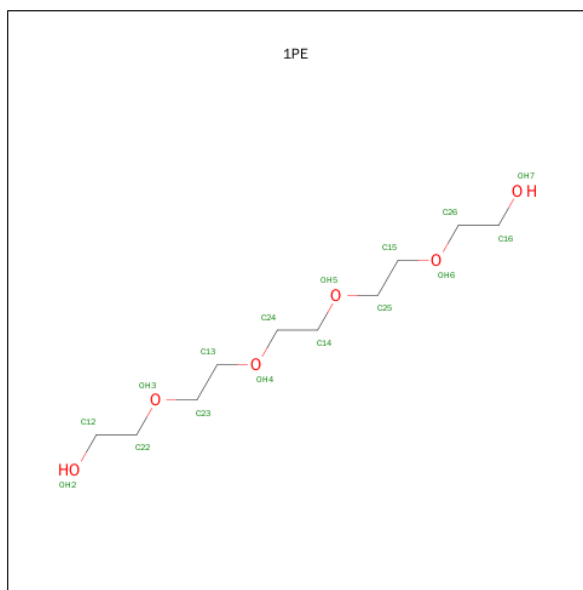
- Molecule 4 is (2S)-2-[[[(R)-[(R)-amino(phenyl)methyl](hydroxy)phosphoryl]methyl]-4-methylpentanoic acid (three-letter code: 4ZN) (formula: C<sub>14</sub>H<sub>22</sub>NO<sub>4</sub>P).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			16	10	1	4	1		
4	B	1	Total	C	N	O	P	0	0
			16	10	1	4	1		
4	C	1	Total	C	N	O	P	0	0
			16	10	1	4	1		
4	D	1	Total	C	N	O	P	0	0
			20	14	1	4	1		
4	E	1	Total	C	N	O	P	0	0
			20	14	1	4	1		
4	F	1	Total	C	N	O	P	0	0
			16	10	1	4	1		
4	G	1	Total	C	N	O	P	0	0
			16	10	1	4	1		
4	H	1	Total	C	N	O	P	0	0
			16	10	1	4	1		
4	I	1	Total	C	N	O	P	0	0
			12	8	1	2	1		
4	J	1	Total	C	N	O	P	0	0
			16	10	1	4	1		
4	K	1	Total	C	N	O	P	0	0
			14	10	1	2	1		
4	L	1	Total	C	N	O	P	0	0
			16	10	1	4	1		

- Molecule 5 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C<sub>10</sub>H<sub>22</sub>O<sub>6</sub>).



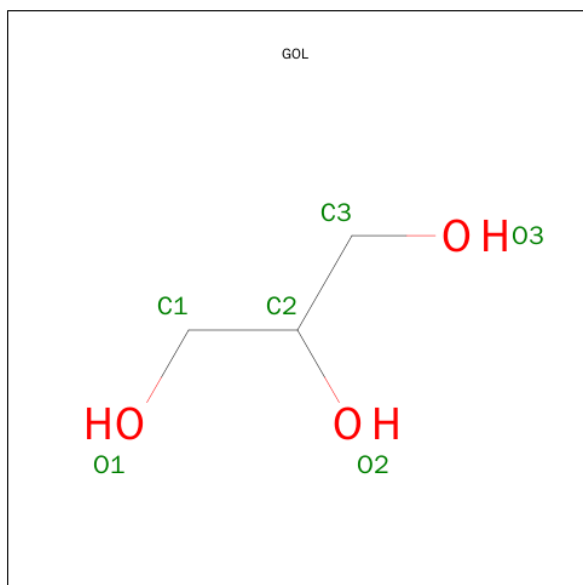
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 9 6 3	0	0
5	A	1	Total C O 12 8 4	0	0
5	B	1	Total C O 10 7 3	0	0
5	B	1	Total C O 10 7 3	0	0
5	C	1	Total C O 13 9 4	0	0
5	C	1	Total C O 9 6 3	0	0
5	D	1	Total C O 10 7 3	0	0
5	D	1	Total C O 10 7 3	0	0
5	E	1	Total C O 12 8 4	0	0
5	E	1	Total C O 12 8 4	0	0
5	F	1	Total C O 10 6 4	0	0
5	G	1	Total C O 9 6 3	0	0
5	G	1	Total C O 6 4 2	0	0
5	G	1	Total C O 6 4 2	0	0
5	H	1	Total C O 10 7 3	0	0
5	H	1	Total C O 10 7 3	0	0
5	I	1	Total C O 12 8 4	0	0
5	I	1	Total C O 11 8 3	0	0
5	J	1	Total C O 11 7 4	0	0
5	J	1	Total C O 11 7 4	0	0
5	J	1	Total C O 10 6 4	0	0
5	K	1	Total C O 12 8 4	0	0

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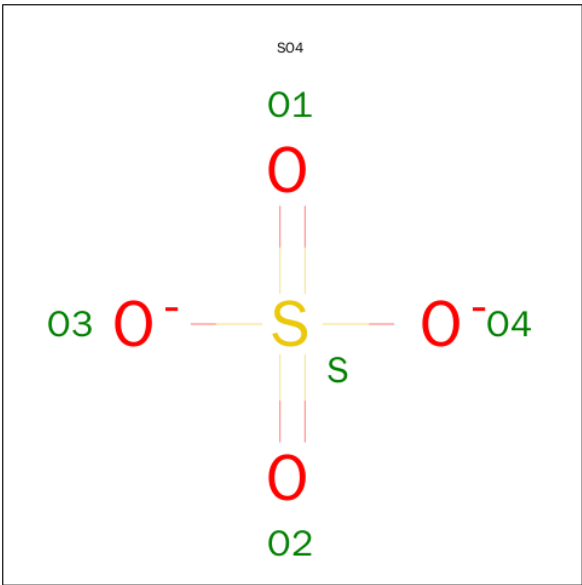
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	K	1	Total	C	O	0	0
			12	8	4		
5	L	1	Total	C	O	0	0
			7	4	3		
5	L	1	Total	C	O	0	0
			10	6	4		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	D	1	Total	O	S	0	0
			5	4	1		
7	E	1	Total	O	S	0	0
			5	4	1		
7	E	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	E	1	Total O S 5 4 1	0	0
7	F	1	Total O S 5 4 1	0	0
7	F	1	Total O S 5 4 1	0	0
7	G	1	Total O S 5 4 1	0	0
7	G	1	Total O S 5 4 1	0	0
7	G	1	Total O S 5 4 1	0	0
7	G	1	Total O S 5 4 1	0	0
7	I	1	Total O S 5 4 1	0	0
7	I	1	Total O S 5 4 1	0	0
7	J	1	Total O S 5 4 1	0	0
7	J	1	Total O S 5 4 1	0	0
7	K	1	Total O S 5 4 1	0	0
7	K	1	Total O S 5 4 1	0	0
7	L	1	Total O S 5 4 1	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	265	Total O 265 265	0	0
8	B	246	Total O 246 246	0	0
8	C	277	Total O 277 277	0	0
8	D	283	Total O 283 283	0	0
8	E	322	Total O 322 322	0	0

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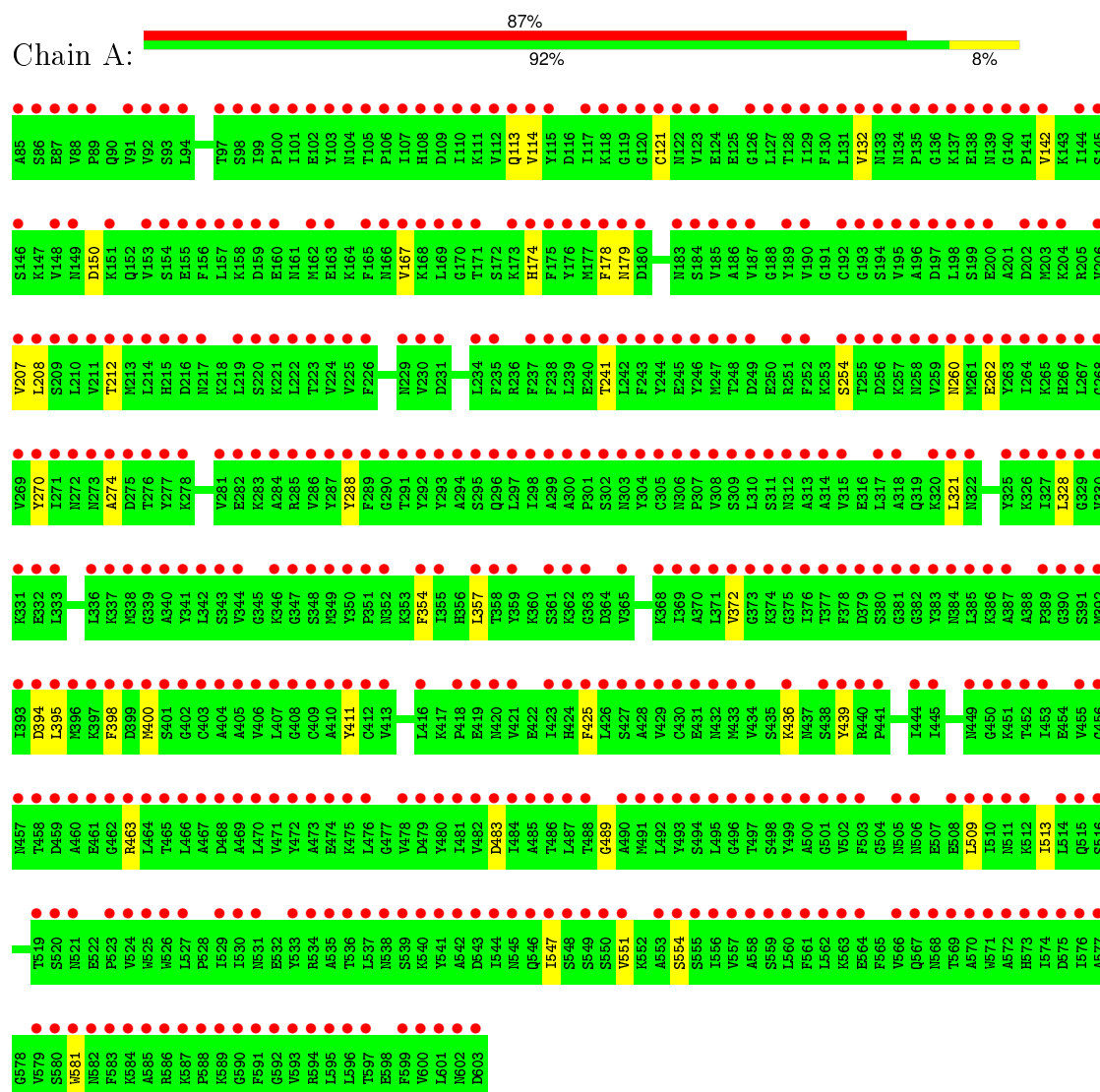
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	F	245	Total 245	O 245	0	0
8	G	281	Total 281	O 281	0	0
8	H	220	Total 220	O 220	0	0
8	I	272	Total 272	O 272	0	0
8	J	287	Total 287	O 287	0	0
8	K	283	Total 283	O 283	0	0
8	L	240	Total 240	O 240	0	0

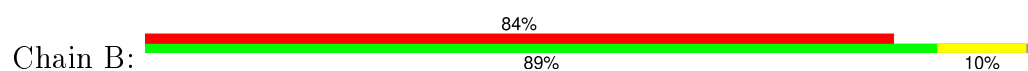
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $\text{RSRZ} > 2$ ). 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: M17 family aminopeptidase

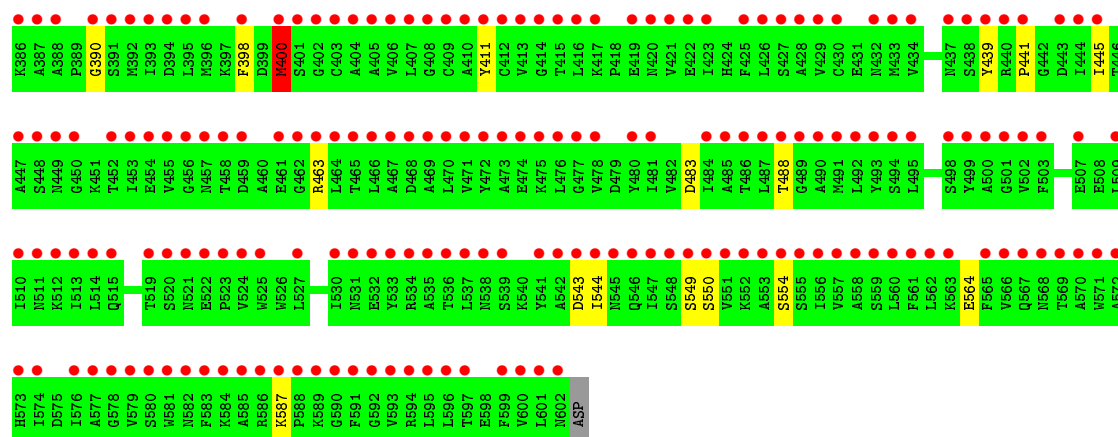


#### • Molecule 1: M17 family aminopeptidase

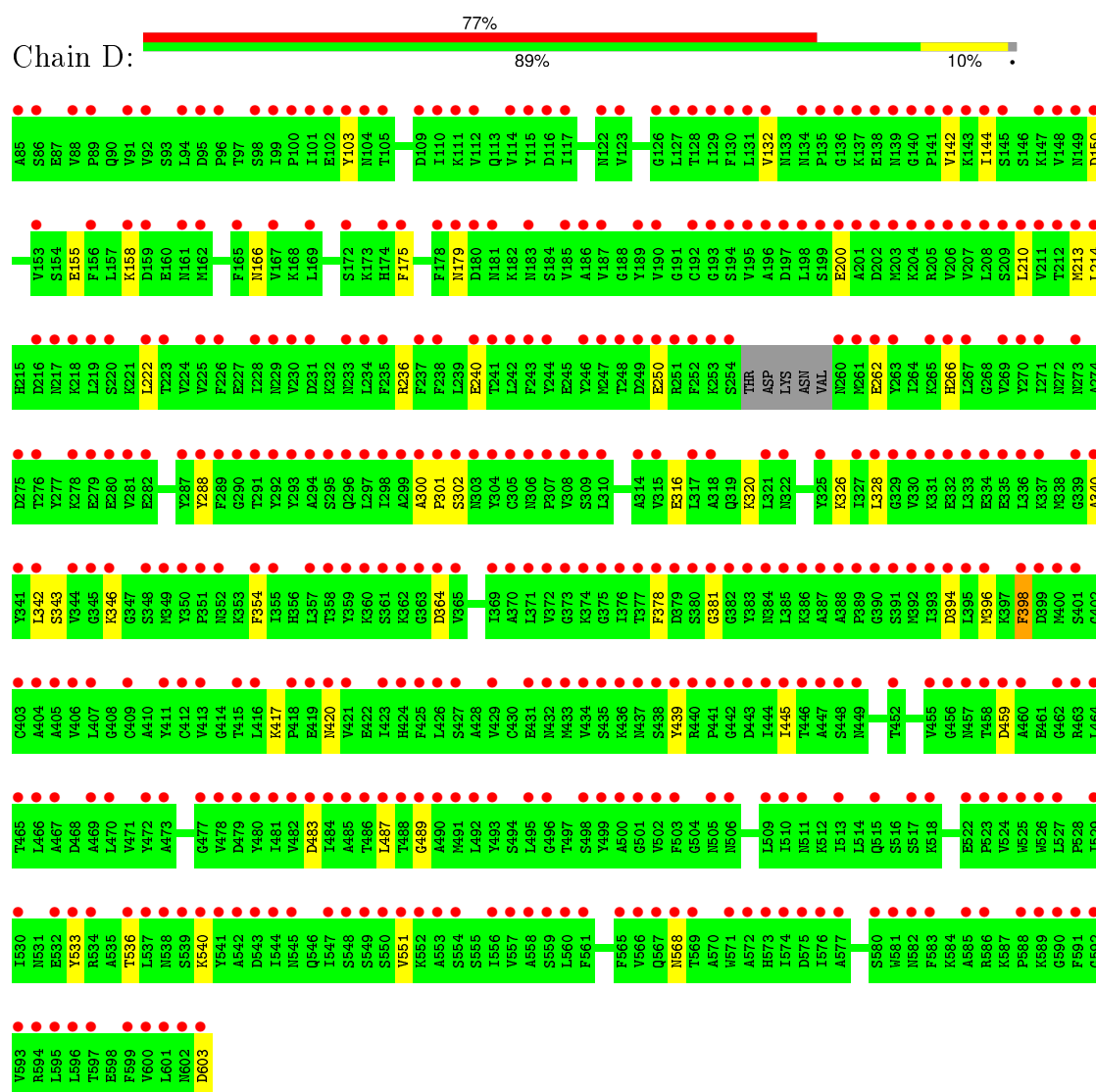






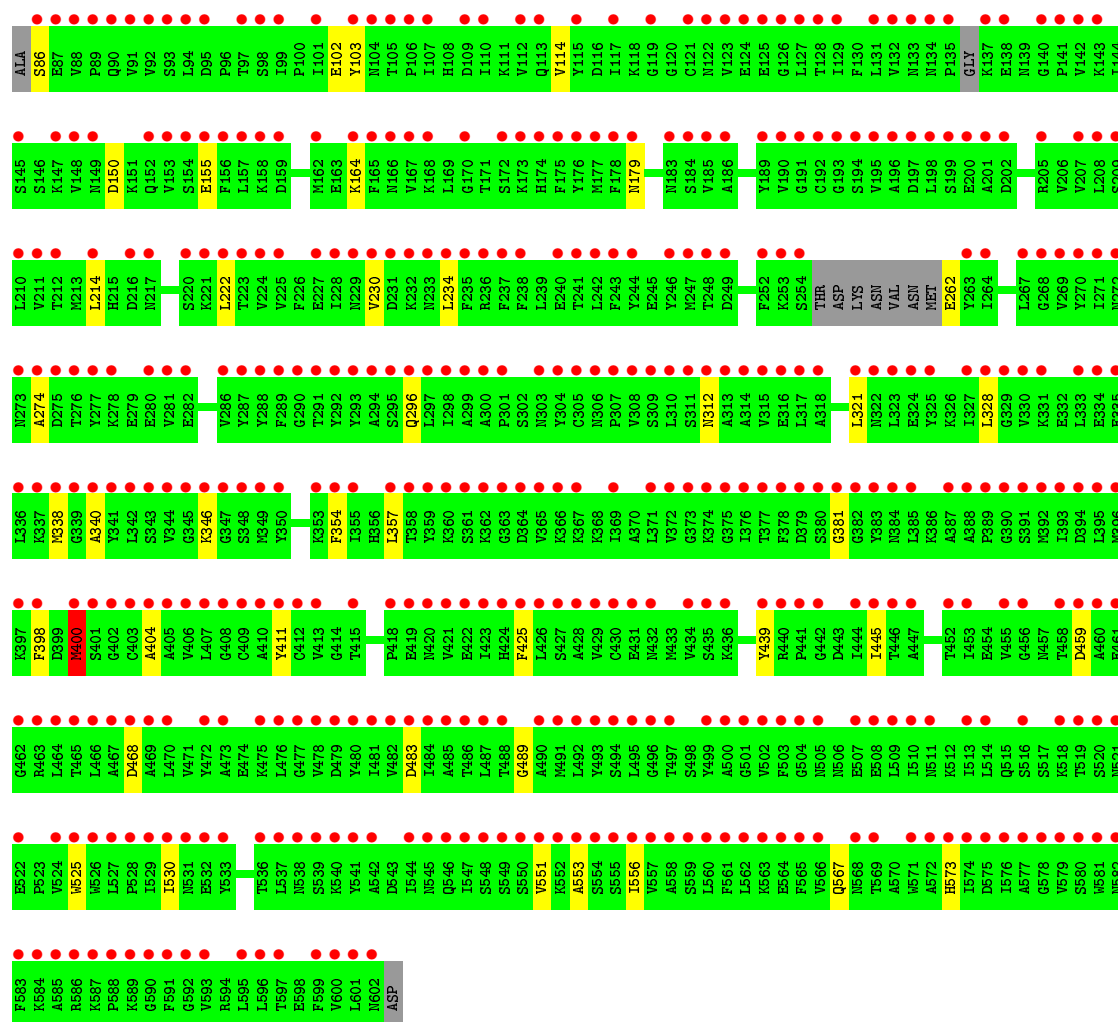


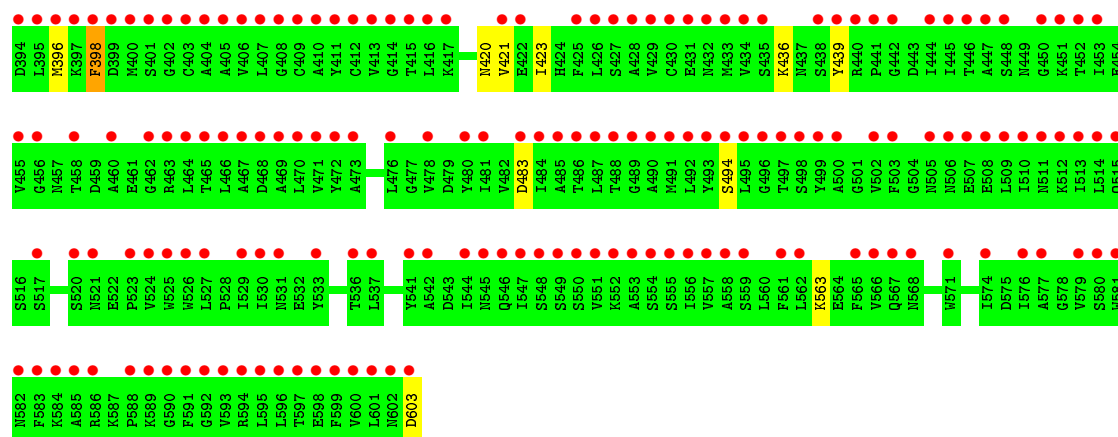
• Molecule 1: M17 family aminopeptidase



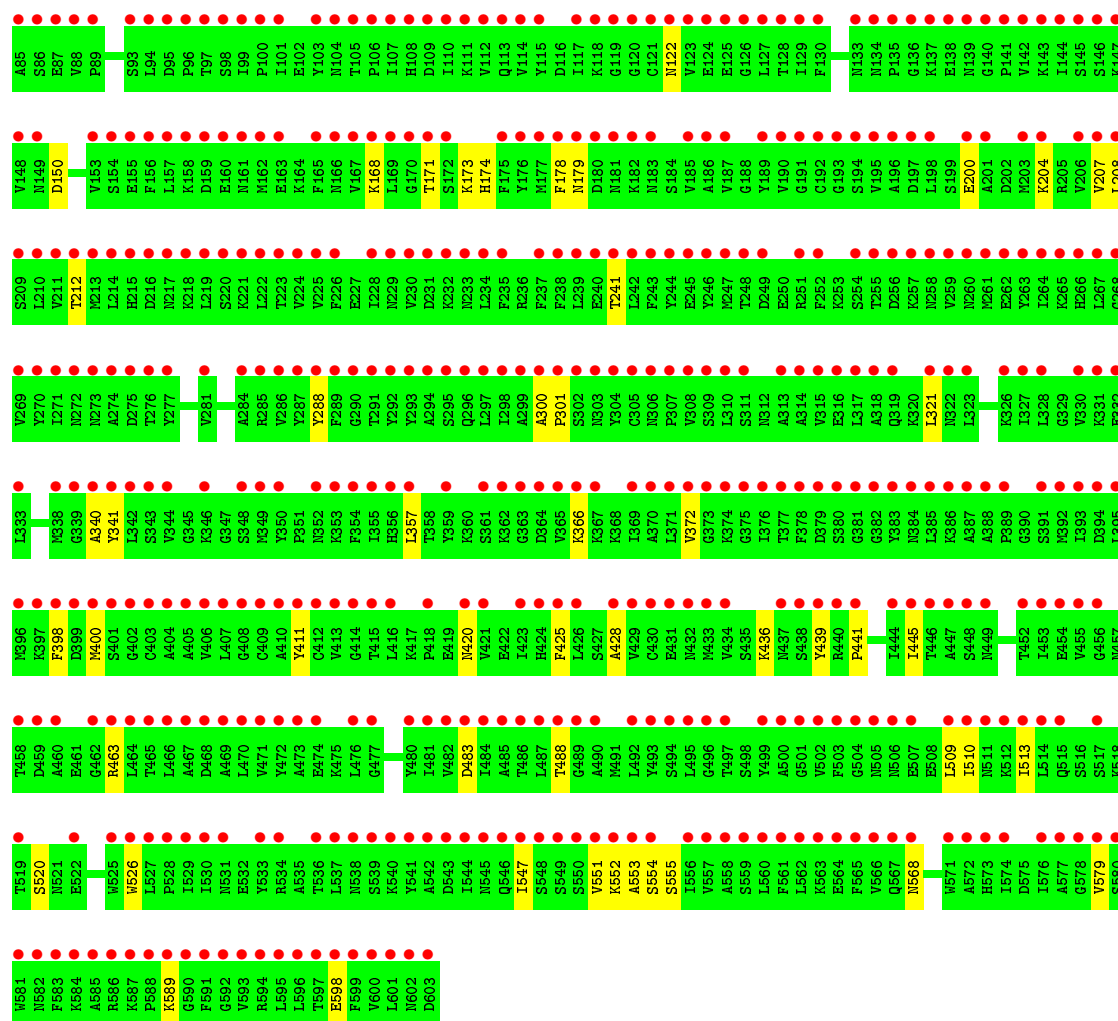
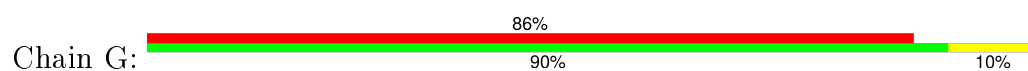
• Molecule 1: M17 family aminopeptidase



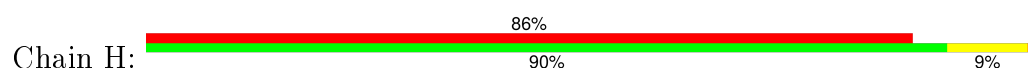


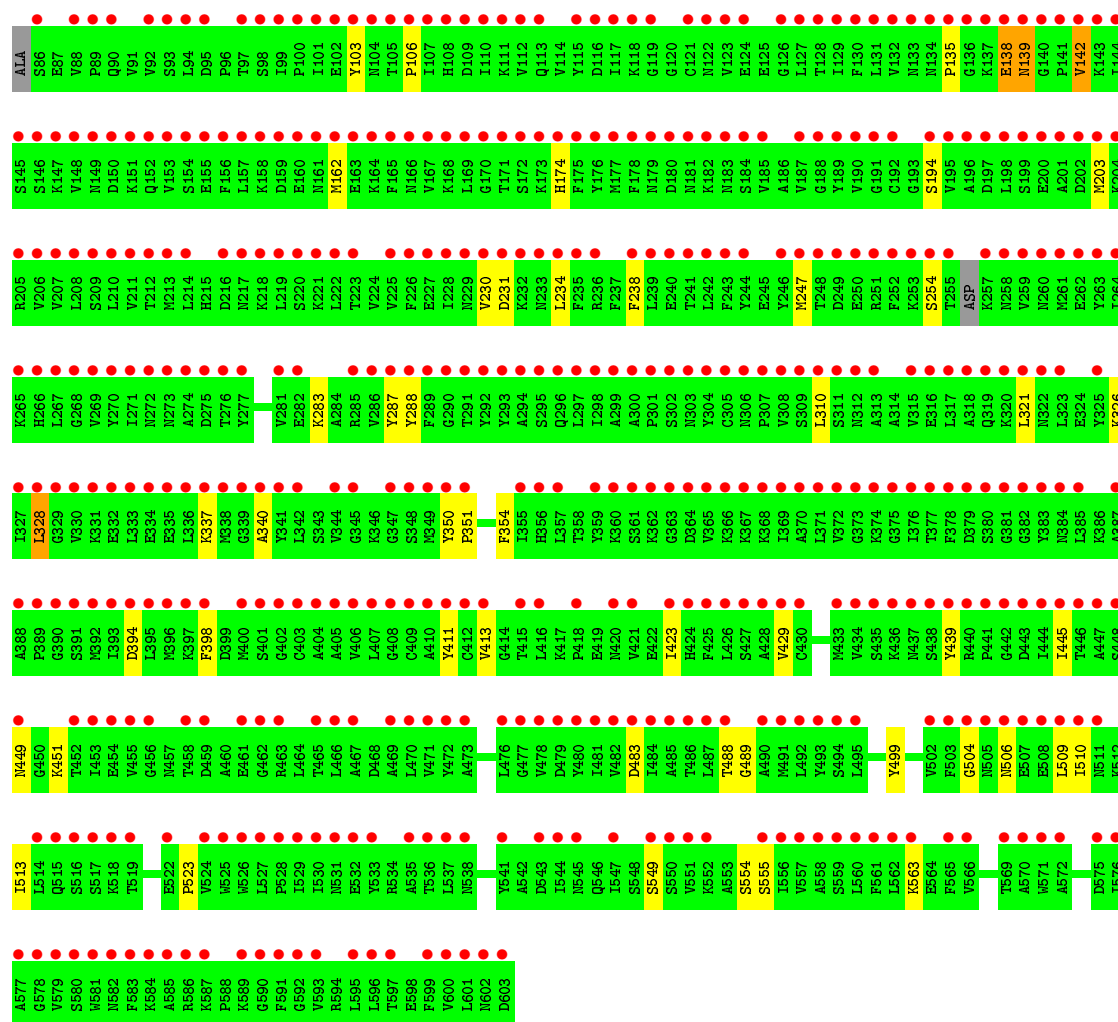


• Molecule 1: M17 family aminopeptidase



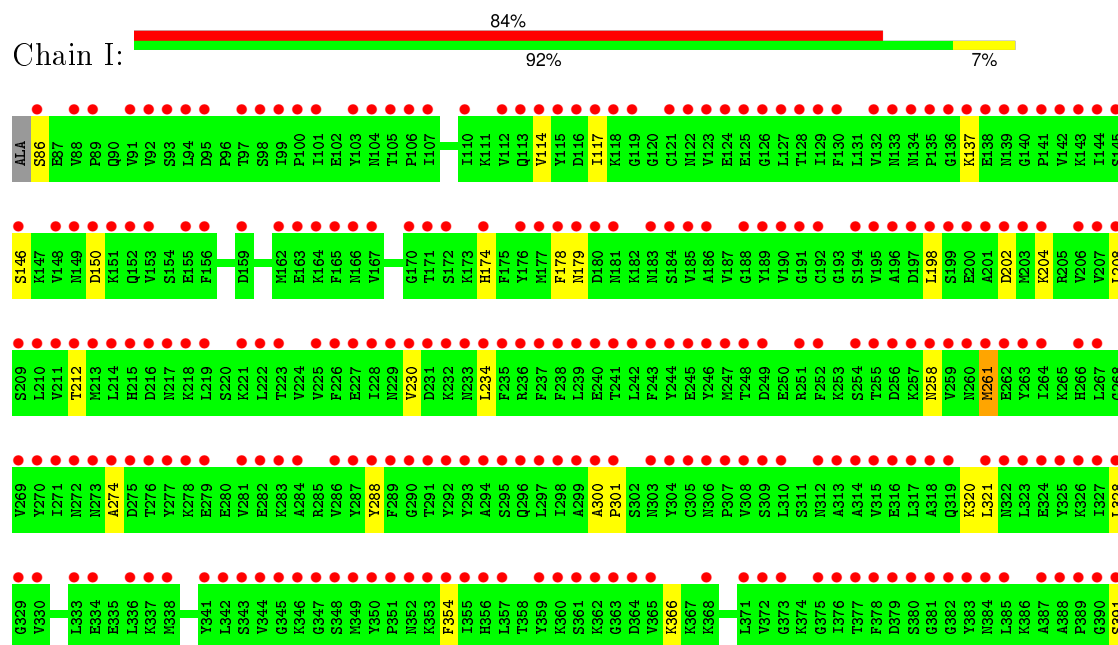
• Molecule 1: M17 family aminopeptidase

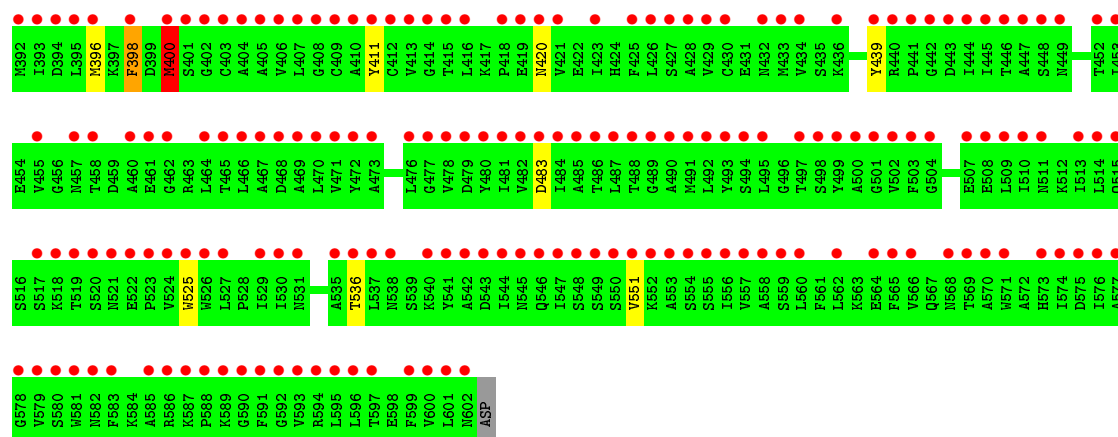




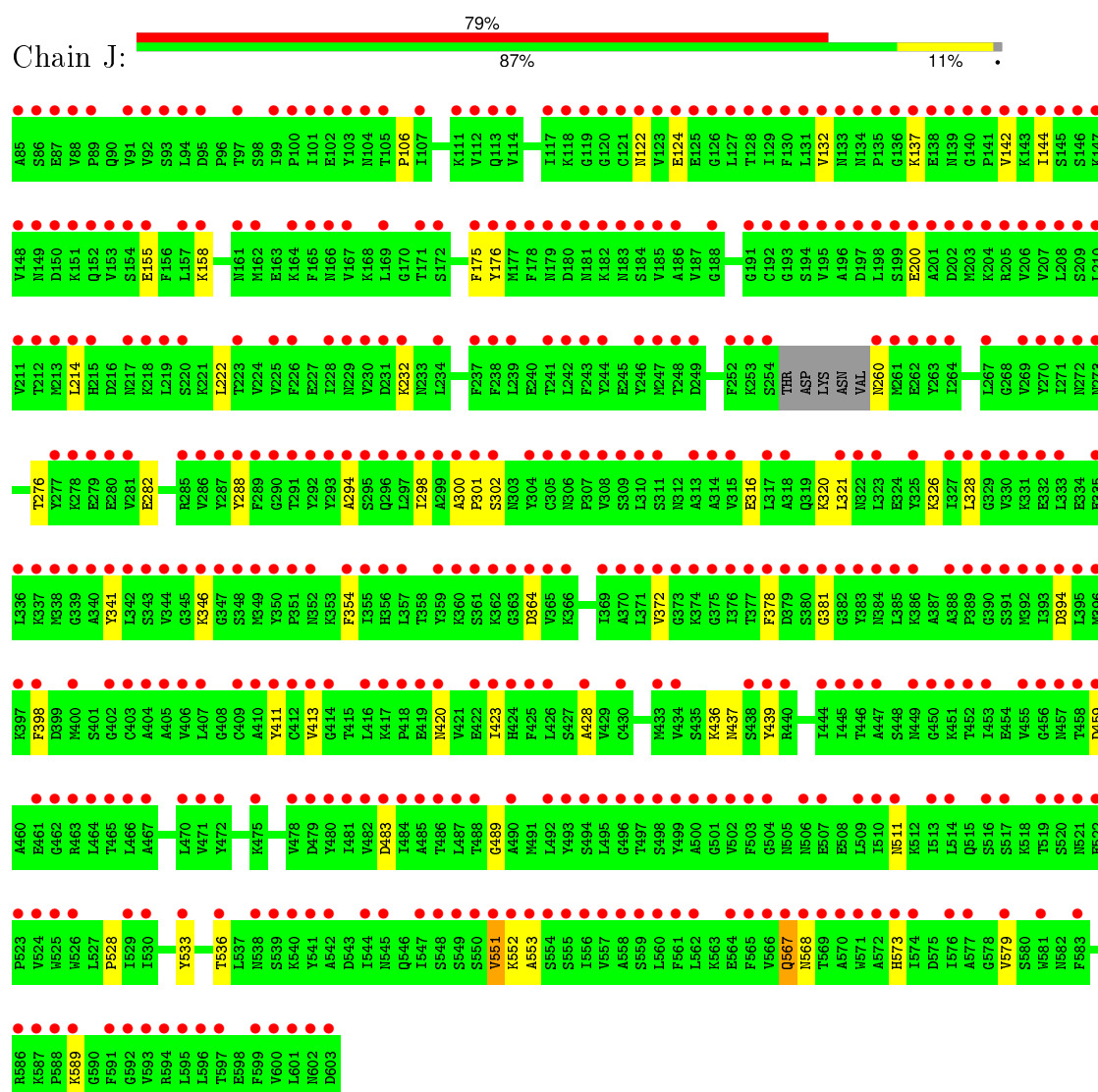
● Molecule 1: M17 family aminopeptidase

Chain I:

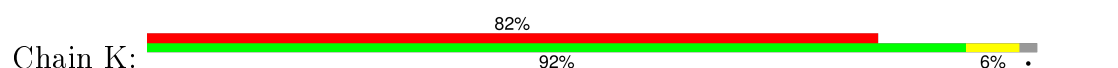


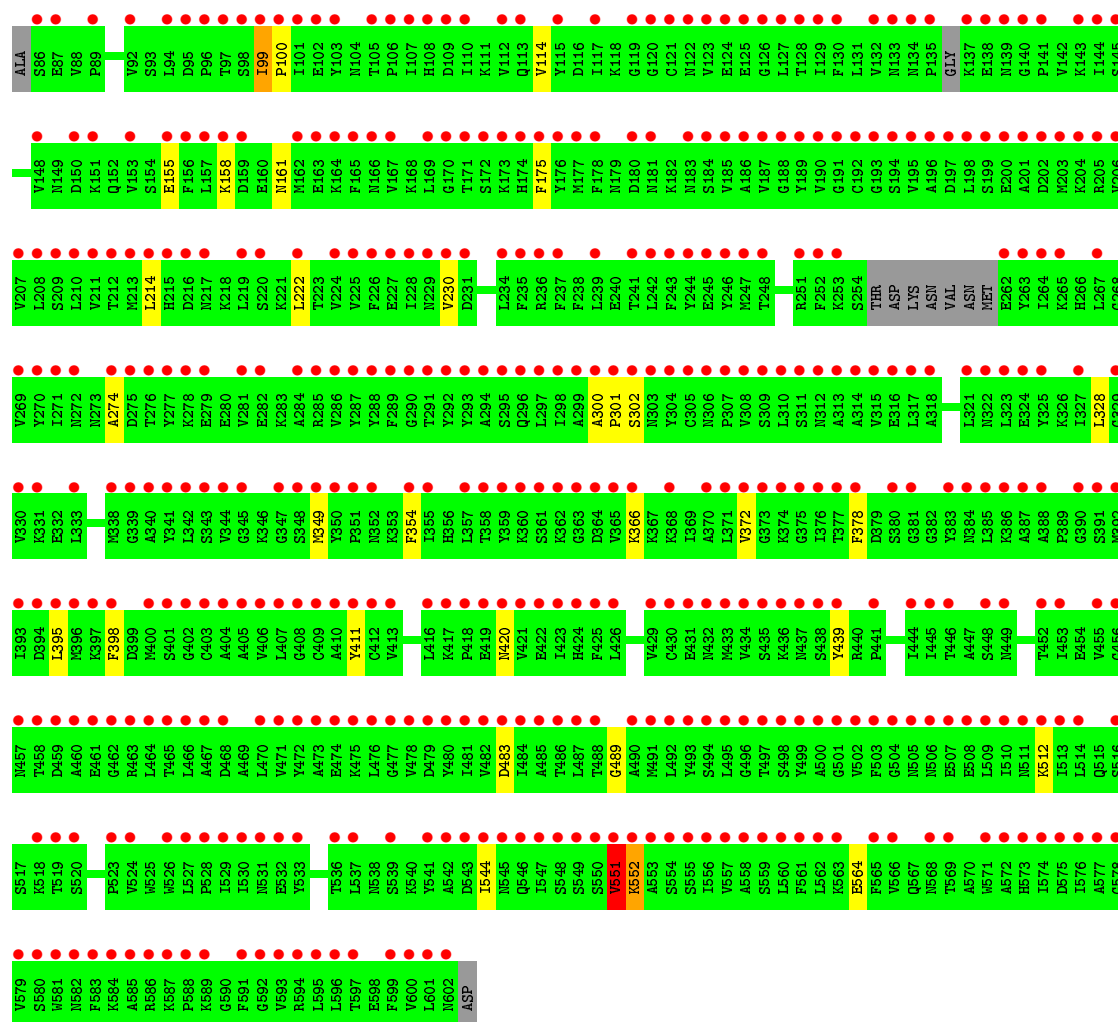


• Molecule 1: M17 family aminopeptidase



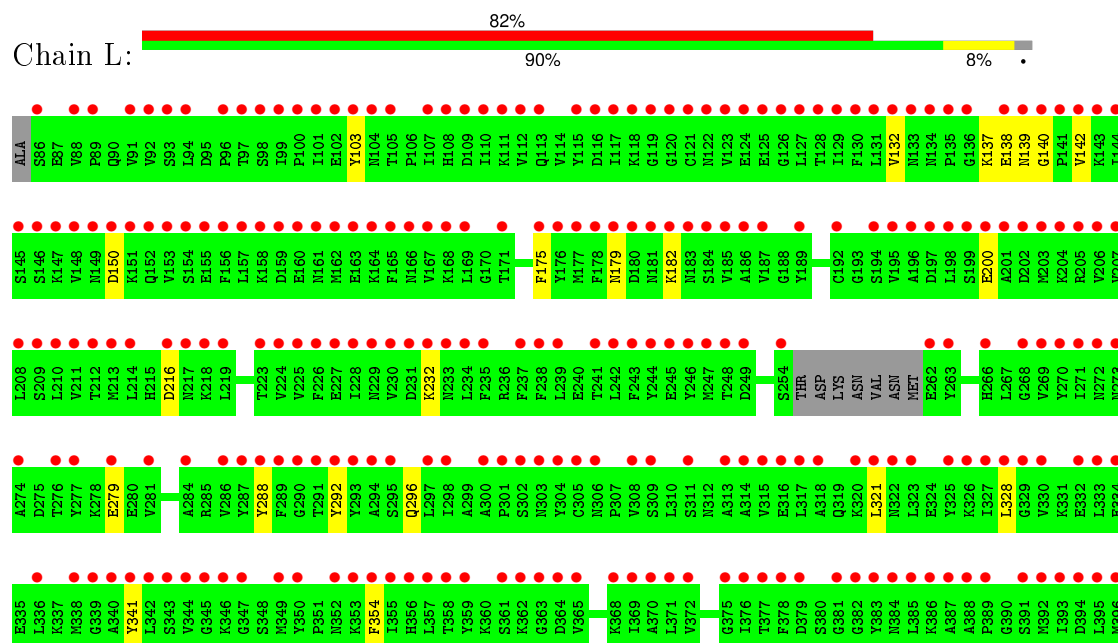
• Molecule 1: M17 family aminopeptidase





• Molecule 1: M17 family aminopeptidase

Chain L:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	174.09Å 177.73Å 230.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.98 – 2.30 48.98 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.98-2.30) 99.9 (48.98-2.30)	Depositor EDS
$R_{merge}$	0.48	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.98 (at 2.29Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.182 , 0.235 0.422 , 0.435	Depositor DCC
$R_{free}$ test set	2920 reflections (0.93%)	DCC
Wilson B-factor (Å <sup>2</sup> )	64.1	Xtriage
Anisotropy	0.534	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 24.6	EDS
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.39$	Xtriage
Outliers	112 of 315398 reflections (0.036%)	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	50850	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.83 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.6001e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, CO3, 1PE, SO4, 4ZN

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	0.43	0/4052	0.55	0/5502
1	B	0.40	0/3979	0.52	0/5405
1	C	0.43	0/4019	0.55	1/5456 (0.0%)
1	D	0.44	0/3997	0.54	0/5422
1	E	0.43	0/3969	0.56	1/5384 (0.0%)
1	F	0.40	0/3928	0.53	0/5342
1	G	0.42	0/4052	0.53	0/5497
1	H	0.39	0/3979	0.52	0/5407
1	I	0.41	0/4029	0.54	1/5466 (0.0%)
1	J	0.43	0/4003	0.54	0/5430
1	K	0.42	0/3960	0.58	1/5372 (0.0%)
1	L	0.41	0/3925	0.54	0/5338
All	All	0.42	0/47892	0.54	4/65021 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	K	0	2
1	L	0	1
All	All	0	3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	99	ILE	C-N-CD	-13.20	91.55	120.60
1	I	400	MET	CA-CB-CG	-7.64	100.31	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	400	MET	CA-CB-CG	-6.05	103.01	113.30
1	C	400	MET	CA-CB-CG	-5.85	103.35	113.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	K	551	VAL	Peptide
1	K	99	ILE	Peptide
1	L	551	VAL	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	3971	0	3875	26	0
1	B	3902	0	3787	29	0
1	C	3941	0	3855	25	0
1	D	3920	0	3851	31	0
1	E	3893	0	3820	26	0
1	F	3851	0	3726	21	0
1	G	3974	0	3899	31	0
1	H	3902	0	3774	31	0
1	I	3951	0	3877	22	0
1	J	3926	0	3854	45	0
1	K	3884	0	3805	18	0
1	L	3848	0	3716	32	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0
2	E	4	0	0	0	0
2	F	4	0	0	0	0
2	G	4	0	0	0	0
2	H	4	0	0	0	0
2	I	4	0	0	0	0
2	J	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	4	0	0	0	0
2	L	4	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
3	I	2	0	0	0	0
3	J	2	0	0	0	0
3	K	2	0	0	0	0
3	L	2	0	0	0	0
4	A	16	0	9	2	0
4	B	16	0	9	3	0
4	C	16	0	9	1	0
4	D	20	0	20	3	0
4	E	20	0	19	2	0
4	F	16	0	9	0	0
4	G	16	0	9	0	0
4	H	16	0	9	1	0
4	I	12	0	7	0	0
4	J	16	0	9	2	0
4	K	14	0	9	1	0
4	L	16	0	9	1	0
5	A	21	0	22	0	0
5	B	20	0	20	3	0
5	C	22	0	24	1	0
5	D	20	0	20	2	0
5	E	24	0	28	2	0
5	F	10	0	13	0	0
5	G	21	0	20	4	0
5	H	20	0	20	1	0
5	I	23	0	26	2	0
5	J	32	0	39	12	0
5	K	24	0	28	2	0
5	L	17	0	21	6	0
6	A	6	0	8	0	0
7	A	25	0	0	2	0
7	B	5	0	0	0	0
7	C	25	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	5	0	0	1	0
7	E	15	0	0	1	0
7	F	10	0	0	0	0
7	G	20	0	0	2	0
7	I	10	0	0	0	0
7	J	10	0	0	0	0
7	K	10	0	0	0	0
7	L	5	0	0	0	0
8	A	265	0	0	3	0
8	B	246	0	0	3	0
8	C	277	0	0	2	0
8	D	283	0	0	5	0
8	E	322	0	0	5	0
8	F	245	0	0	4	0
8	G	281	0	0	0	0
8	H	220	0	0	2	0
8	I	272	0	0	3	0
8	J	287	0	0	5	0
8	K	283	0	0	1	0
8	L	240	0	0	4	0
All	All	50850	0	46255	326	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 3.

All (326) 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:J:320:LYS:HZ1	5:J:706:1PE:H151	1.30	0.96
1:J:489:GLY:N	4:J:704:4ZN:O20	2.06	0.88
1:L:532:GLU:HB2	5:L:705:1PE:H142	1.55	0.87
1:H:328:LEU:HB2	1:H:354:PHE:HB3	1.65	0.78
1:B:320:LYS:HZ1	5:B:706:1PE:H241	1.50	0.77
1:B:504:GLY:HA3	1:B:510:ILE:HD11	1.68	0.76
1:F:563:LYS:NZ	8:F:802:HOH:O	2.19	0.76
1:J:320:LYS:HZ1	5:J:706:1PE:H141	1.51	0.75
4:B:704:4ZN:H20	4:B:704:4ZN:H16	1.69	0.73
1:H:139:ASN:HD22	1:H:139:ASN:N	1.86	0.73
1:I:178:PHE:HZ	1:K:155:GLU:HG2	1.55	0.71
1:E:489:GLY:N	4:E:704:4ZN:O20	2.21	0.70
1:C:411:TYR:HE1	5:C:706:1PE:H232	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:320:LYS:NZ	5:J:706:1PE:H151	2.07	0.69
1:B:340:ALA:HA	1:B:445:ILE:HD12	1.74	0.68
1:A:132:VAL:HG21	1:A:142:VAL:HG13	1.76	0.68
1:C:587:LYS:NZ	8:C:802:HOH:O	2.24	0.67
1:L:132:VAL:HG21	1:L:142:VAL:HG13	1.74	0.67
1:A:260:ASN:O	8:A:801:HOH:O	2.12	0.67
1:B:332:GLU:OE2	8:B:801:HOH:O	2.13	0.66
1:E:262:GLU:N	8:E:805:HOH:O	2.27	0.66
5:J:705:1PE:H242	1:L:451:LYS:HE3	1.77	0.66
1:B:328:LEU:HB2	1:B:354:PHE:HB3	1.78	0.65
1:L:216:ASP:OD1	8:L:801:HOH:O	2.15	0.65
1:K:411:TYR:HE1	5:K:706:1PE:H241	1.62	0.65
1:E:230:VAL:HG22	1:E:234:LEU:HD23	1.79	0.64
1:A:113:GLN:NE2	8:A:805:HOH:O	2.31	0.64
1:D:603:ASP:O	8:D:802:HOH:O	2.15	0.64
1:F:328:LEU:HB2	1:F:354:PHE:HB3	1.79	0.64
1:G:122:ASN:HD22	5:G:706:1PE:H142	1.64	0.63
1:D:417:LYS:O	8:D:801:HOH:O	2.15	0.63
1:L:138:GLU:N	1:L:139:ASN:HA	2.13	0.63
1:B:248:THR:HG21	1:B:261:MET:HE1	1.81	0.63
4:D:704:4ZN:O20	8:D:803:HOH:O	2.16	0.62
1:I:366:LYS:HG3	1:I:420:ASN:HB3	1.80	0.62
1:A:463:ARG:NH1	7:A:712:SO4:O3	2.30	0.62
1:F:190:VAL:HG11	1:F:206:VAL:HG13	1.83	0.61
1:J:282:GLU:OE1	8:J:801:HOH:O	2.16	0.61
1:E:114:VAL:HG12	1:E:274:ALA:HB1	1.81	0.61
1:J:132:VAL:HG21	1:J:142:VAL:HG13	1.82	0.61
1:J:122:ASN:OD1	1:J:124:GLU:HG2	2.01	0.60
1:D:132:VAL:HG21	1:D:142:VAL:HG13	1.83	0.60
1:F:603:ASP:O	8:F:801:HOH:O	2.17	0.60
1:L:182:LYS:O	8:L:802:HOH:O	2.16	0.59
1:E:164:LYS:NZ	8:E:810:HOH:O	2.35	0.59
1:J:328:LEU:HB2	1:J:354:PHE:HB3	1.83	0.59
1:K:489:GLY:H	4:K:704:4ZN:C19	2.16	0.59
1:H:489:GLY:N	4:H:704:4ZN:O20	2.30	0.58
1:H:138:GLU:C	1:H:139:ASN:HD22	2.07	0.58
1:F:137:LYS:CB	1:F:140:GLY:H	2.16	0.58
1:E:411:TYR:HE1	5:E:706:1PE:H241	1.68	0.58
1:D:214:LEU:HD21	1:D:222:LEU:HD22	1.85	0.58
1:L:551:VAL:HA	1:L:552:LYS:CB	2.33	0.58
1:K:328:LEU:HB2	1:K:354:PHE:HB3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:137:LYS:CB	1:L:140:GLY:H	2.18	0.57
1:H:230:VAL:HG12	1:H:234:LEU:HD23	1.85	0.57
1:G:208:LEU:O	1:G:212:THR:HG23	2.05	0.57
1:B:103:TYR:CD2	5:B:706:1PE:H132	2.40	0.57
1:D:533:TYR:O	1:D:536:THR:HG22	2.05	0.57
1:F:176:TYR:OH	1:F:217:ASN:OD1	2.13	0.57
1:E:483:ASP:OD1	1:E:573:HIS:ND1	2.35	0.57
1:H:504:GLY:HA3	1:H:510:ILE:HD11	1.87	0.57
1:K:411:TYR:CE1	5:K:706:1PE:H241	2.40	0.57
1:D:487:LEU:O	4:D:704:4ZN:H17	2.04	0.57
1:J:436:LYS:HG3	1:K:349:MET:HB3	1.85	0.57
1:G:321:LEU:HD11	1:G:411:TYR:HA	1.86	0.57
1:C:275:ASP:HA	1:C:278:LYS:HG3	1.86	0.57
1:L:530:ILE:HA	5:L:705:1PE:H152	1.86	0.56
1:G:178:PHE:HZ	1:J:155:GLU:HG2	1.70	0.56
1:C:321:LEU:HD11	1:C:411:TYR:HA	1.88	0.56
1:C:400:MET:HE2	1:C:400:MET:O	2.05	0.56
1:G:207:VAL:HG11	1:G:241:THR:HG22	1.87	0.56
1:E:530:ILE:HD12	1:E:556:ILE:HD13	1.88	0.56
1:L:232:LYS:NZ	1:L:279:GLU:OE2	2.31	0.56
1:A:207:VAL:HG11	1:A:241:THR:HG22	1.87	0.56
1:B:207:VAL:HG11	1:B:241:THR:HG22	1.86	0.55
1:D:328:LEU:HB2	1:D:354:PHE:HB3	1.89	0.55
1:H:142:VAL:HG22	1:H:162:MET:HB3	1.89	0.55
1:D:340:ALA:HA	1:D:445:ILE:HD12	1.89	0.55
1:K:114:VAL:HG12	1:K:274:ALA:HB1	1.88	0.55
1:C:178:PHE:HZ	1:E:155:GLU:HG2	1.72	0.55
1:L:530:ILE:HG23	5:L:705:1PE:H141	1.89	0.54
5:J:705:1PE:H261	1:L:543:ASP:HB3	1.88	0.54
1:C:90:GLN:HB3	1:C:95:ASP:HB2	1.90	0.54
1:I:391:SER:OG	8:I:801:HOH:O	2.17	0.54
1:A:489:GLY:N	4:A:704:4ZN:O21	2.35	0.54
1:A:328:LEU:HB2	1:A:354:PHE:HB3	1.90	0.54
1:F:132:VAL:HG21	1:F:142:VAL:HG13	1.89	0.54
1:J:533:TYR:O	1:J:536:THR:HG22	2.08	0.53
1:H:174:HIS:HB3	1:L:175:PHE:CD2	2.43	0.53
5:J:705:1PE:H262	1:L:451:LYS:HG2	1.89	0.53
1:G:411:TYR:HE1	5:G:705:1PE:H131	1.73	0.53
1:D:394:ASP:OD1	1:D:394:ASP:N	2.35	0.53
1:A:260:ASN:ND2	1:D:166:ASN:HB3	2.24	0.53
1:A:547:ILE:HA	7:A:712:SO4:O3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:579:VAL:O	1:J:589:LYS:HD2	2.09	0.53
1:J:316:GLU:HG3	5:J:706:1PE:H262	1.89	0.53
1:H:103:TYR:CD2	5:H:705:1PE:H221	2.43	0.53
1:B:528:PRO:HB3	1:E:525:TRP:CZ3	2.44	0.52
1:I:258:ASN:HB3	1:I:261:MET:HB2	1.91	0.52
1:H:139:ASN:N	1:H:139:ASN:ND2	2.57	0.52
1:B:506:ASN:O	1:B:510:ILE:HG12	2.09	0.52
1:I:174:HIS:NE2	8:I:810:HOH:O	2.32	0.52
1:E:86:SER:HB2	1:E:312:ASN:OD1	2.10	0.52
1:J:132:VAL:HG11	1:J:144:ILE:HD13	1.91	0.52
1:H:413:VAL:HG11	1:H:423:ILE:HD13	1.92	0.52
1:C:390:GLY:N	7:C:708:SO4:O2	2.43	0.51
1:J:260:ASN:N	8:J:808:HOH:O	2.42	0.51
1:B:320:LYS:NZ	5:B:706:1PE:H241	2.23	0.51
1:L:567:GLN:HG3	8:L:986:HOH:O	2.10	0.51
1:A:395:LEU:HD11	1:A:581:TRP:CD1	2.45	0.51
1:J:394:ASP:HA	1:L:441:PRO:HB2	1.92	0.51
1:D:103:TYR:N	7:D:707:SO4:O3	2.30	0.51
1:A:208:LEU:O	1:A:212:THR:HG23	2.10	0.51
1:I:198:LEU:HD22	1:I:202:ASP:HB3	1.92	0.51
5:J:705:1PE:H262	1:L:451:LYS:HE2	1.93	0.51
1:G:178:PHE:CZ	1:J:155:GLU:HG2	2.46	0.50
1:F:122:ASN:HB3	8:F:966:HOH:O	2.11	0.50
1:G:122:ASN:ND2	5:G:706:1PE:H142	2.25	0.50
1:E:346:LYS:NZ	8:E:808:HOH:O	2.33	0.50
1:H:563:LYS:HE2	8:H:870:HOH:O	2.11	0.50
1:D:302:SER:OG	1:D:378:PHE:HB2	2.12	0.50
1:G:551:VAL:HG12	1:G:553:ALA:H	1.76	0.50
1:J:326:LYS:NZ	8:J:810:HOH:O	2.45	0.49
1:F:221:LYS:HG3	1:F:266:HIS:HB2	1.93	0.49
1:E:328:LEU:HB2	1:E:354:PHE:HB3	1.94	0.49
1:B:520:SER:HB3	1:B:598:GLU:HG3	1.92	0.49
1:C:112:VAL:HG22	1:C:267:LEU:HB3	1.95	0.49
1:L:139:ASN:N	8:L:810:HOH:O	2.43	0.49
1:D:316:GLU:HG3	5:D:705:1PE:H221	1.95	0.49
1:A:174:HIS:HB3	1:D:175:PHE:CD2	2.48	0.49
1:G:463:ARG:NH1	7:G:711:SO4:O2	2.45	0.49
1:A:150:ASP:OD2	1:A:179:ASN:HB2	2.12	0.49
1:E:551:VAL:HG12	1:E:553:ALA:H	1.77	0.49
1:A:372:VAL:O	1:A:483:ASP:HA	2.13	0.49
1:L:489:GLY:N	4:L:704:4ZN:O21	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:GLN:HB3	1:B:95:ASP:HB2	1.95	0.49
1:F:138:GLU:N	1:F:139:ASN:HA	2.27	0.48
1:C:117:ILE:HD13	1:C:270:TYR:HB3	1.95	0.48
1:A:254:SER:HB3	1:C:543:ASP:OD2	2.13	0.48
1:I:178:PHE:CZ	1:K:155:GLU:HG2	2.43	0.48
1:J:321:LEU:HD11	1:J:411:TYR:HA	1.94	0.48
1:B:322:ASN:HB2	8:B:1011:HOH:O	2.13	0.48
1:I:230:VAL:HG12	1:I:234:LEU:HD23	1.95	0.48
1:D:540:LYS:NZ	8:D:811:HOH:O	2.43	0.48
1:G:520:SER:HB3	1:G:598:GLU:HG3	1.95	0.48
4:E:704:4ZN:H20	4:E:704:4ZN:H15	1.96	0.48
1:G:366:LYS:HG3	1:G:420:ASN:HB3	1.96	0.48
1:C:328:LEU:HB2	1:C:354:PHE:HB3	1.95	0.48
1:E:338:MET:HE2	1:E:468:ASP:HB3	1.96	0.48
1:D:266:HIS:ND1	8:D:805:HOH:O	2.23	0.48
1:F:366:LYS:HG3	1:F:420:ASN:HB3	1.96	0.47
1:B:341:TYR:CE1	1:B:428:ALA:HB1	2.49	0.47
1:B:255:THR:HA	8:B:829:HOH:O	2.13	0.47
1:H:340:ALA:HA	1:H:445:ILE:HD12	1.95	0.47
1:D:381:GLY:HA2	1:D:459:ASP:OD1	2.14	0.47
1:F:210:LEU:HA	1:F:213:MET:HE2	1.97	0.47
1:L:328:LEU:HB2	1:L:354:PHE:HB3	1.96	0.47
1:L:531:ASN:H	5:L:705:1PE:H152	1.78	0.47
1:E:567:GLN:OE1	8:E:802:HOH:O	2.20	0.47
1:B:386:LYS:HZ1	4:B:704:4ZN:H16	1.79	0.47
1:L:520:SER:HB3	1:L:598:GLU:HG3	1.96	0.47
1:D:155:GLU:O	1:D:158:LYS:HG2	2.14	0.47
1:K:214:LEU:HD11	1:K:222:LEU:HD22	1.97	0.47
1:A:321:LEU:HD11	1:A:411:TYR:HA	1.97	0.47
4:B:704:4ZN:H20	4:B:704:4ZN:C07	2.43	0.47
1:J:411:TYR:HE1	5:J:707:1PE:H252	1.81	0.46
1:E:338:MET:CE	1:E:468:ASP:HB3	2.45	0.46
1:A:509:LEU:O	1:A:513:ILE:HG12	2.15	0.46
1:B:413:VAL:HG11	1:B:423:ILE:HD12	1.97	0.46
4:J:704:4ZN:O10	4:J:704:4ZN:H20	2.16	0.46
1:H:135:PRO:HA	1:H:194:SER:O	2.16	0.46
1:G:150:ASP:OD2	1:G:179:ASN:HB2	2.15	0.46
1:D:396:MET:SD	1:D:398:PHE:HE2	2.39	0.46
1:G:174:HIS:HB3	1:J:175:PHE:CD2	2.51	0.46
1:A:262:GLU:HA	8:A:835:HOH:O	2.16	0.46
1:J:568:ASN:O	1:J:568:ASN:ND2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:321:LEU:HD11	1:I:411:TYR:HA	1.98	0.45
1:B:460:ALA:HB3	1:B:546:GLN:NE2	2.31	0.45
1:L:341:TYR:CE1	1:L:428:ALA:HB1	2.51	0.45
1:G:372:VAL:O	1:G:483:ASP:HA	2.16	0.45
1:G:300:ALA:HA	1:G:301:PRO:HD3	1.83	0.45
1:G:357:LEU:HB2	1:G:425:PHE:HB2	1.97	0.45
1:B:168:LYS:O	1:B:171:THR:HG22	2.16	0.45
1:K:551:VAL:HA	1:K:552:LYS:CB	2.46	0.45
7:E:707:SO4:O4	1:F:436:LYS:HG2	2.16	0.45
1:I:396:MET:SD	1:I:398:PHE:HE2	2.40	0.45
1:H:142:VAL:CG2	1:H:162:MET:HB3	2.47	0.45
1:I:208:LEU:O	1:I:212:THR:HG23	2.16	0.45
1:J:411:TYR:CE1	5:J:707:1PE:H252	2.52	0.45
1:G:341:TYR:CE1	1:G:428:ALA:HB1	2.51	0.45
1:I:525:TRP:CE2	1:J:528:PRO:HD3	2.51	0.45
1:C:216:ASP:HB3	8:E:916:HOH:O	2.17	0.45
1:D:489:GLY:H	4:D:704:4ZN:H15	1.80	0.45
1:K:372:VAL:O	1:K:483:ASP:HA	2.17	0.45
5:J:706:1PE:H151	5:J:706:1PE:H141	1.67	0.44
1:L:551:VAL:HG12	1:L:553:ALA:H	1.82	0.44
1:H:506:ASN:O	1:H:510:ILE:HG12	2.18	0.44
1:A:394:ASP:HA	1:C:441:PRO:HB2	1.99	0.44
1:H:283:LYS:HE2	1:H:287:TYR:CZ	2.52	0.44
1:D:343:SER:HA	1:D:346:LYS:HD3	1.98	0.44
1:J:232:LYS:HD2	1:J:276:THR:HG22	1.99	0.44
1:B:175:PHE:N	1:B:187:VAL:O	2.41	0.44
1:F:248:THR:HG22	8:F:892:HOH:O	2.17	0.44
1:A:395:LEU:HD11	1:A:581:TRP:CG	2.52	0.44
1:H:509:LEU:O	1:H:513:ILE:HG12	2.18	0.44
1:H:106:PRO:HD2	1:H:247:MET:SD	2.58	0.44
1:I:320:LYS:HE2	5:I:705:1PE:H131	1.99	0.44
1:D:326:LYS:HG2	1:D:328:LEU:HD12	2.00	0.44
1:H:337:LYS:NZ	8:H:821:HOH:O	2.49	0.44
1:J:214:LEU:HD21	1:J:222:LEU:HD22	2.00	0.44
1:C:463:ARG:NH1	7:C:711:SO4:O3	2.48	0.44
1:J:302:SER:OG	1:J:378:PHE:HB2	2.18	0.44
1:G:509:LEU:O	1:G:513:ILE:HG12	2.18	0.44
1:H:321:LEU:HD11	1:H:411:TYR:HA	1.98	0.43
1:L:137:LYS:C	1:L:139:ASN:HA	2.38	0.43
1:A:121:CYS:HA	1:A:270:TYR:CE2	2.53	0.43
1:F:114:VAL:HG12	1:F:274:ALA:HB1	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:204:LYS:HE2	1:I:204:LYS:HB2	1.83	0.43
1:G:436:LYS:HE2	1:G:436:LYS:HB3	1.81	0.43
5:L:705:1PE:H242	5:L:705:1PE:H252	1.83	0.43
1:E:381:GLY:HA2	1:E:459:ASP:OD1	2.17	0.43
1:G:579:VAL:O	1:G:589:LYS:HD2	2.18	0.43
1:E:357:LEU:HB2	1:E:425:PHE:HB2	1.99	0.43
1:E:340:ALA:HA	1:E:445:ILE:HD12	2.00	0.43
1:L:533:TYR:HB2	1:L:560:LEU:HD11	1.99	0.43
1:K:512:LYS:NZ	8:K:814:HOH:O	2.51	0.43
1:L:321:LEU:HD11	1:L:411:TYR:HA	1.99	0.43
1:A:489:GLY:H	4:A:704:4ZN:C19	2.29	0.43
1:G:547:ILE:HB	7:G:711:SO4:O4	2.18	0.43
1:G:168:LYS:HB3	1:G:171:THR:OG1	2.19	0.43
1:C:230:VAL:HG12	1:C:234:LEU:HD23	2.01	0.43
1:J:567:GLN:NE2	8:J:819:HOH:O	2.51	0.43
1:I:114:VAL:HG12	1:I:274:ALA:HB1	2.00	0.43
1:G:441:PRO:HB2	1:H:394:ASP:HA	2.01	0.43
1:I:117:ILE:HD11	1:I:146:SER:OG	2.19	0.43
1:D:236:ARG:O	1:D:240:GLU:HG3	2.18	0.43
1:J:381:GLY:HA2	1:J:459:ASP:OD1	2.18	0.43
1:G:204:LYS:HB2	1:G:204:LYS:HE3	1.78	0.43
1:A:132:VAL:HG23	1:A:167:VAL:HG12	1.99	0.43
1:I:174:HIS:HB3	1:K:175:PHE:CD2	2.54	0.43
1:E:102:GLU:HG2	1:E:296:GLN:OE1	2.18	0.43
1:C:544:ILE:HD12	1:C:564:GLU:HG3	2.00	0.43
1:F:421:VAL:HG22	1:F:423:ILE:HG13	2.00	0.43
1:D:320:LYS:HE2	5:D:705:1PE:H231	2.01	0.43
1:B:350:TYR:HA	1:B:351:PRO:HD3	1.89	0.43
1:D:150:ASP:OD2	1:D:179:ASN:HB2	2.19	0.43
1:K:366:LYS:HG3	1:K:420:ASN:HB3	2.01	0.43
1:H:350:TYR:HA	1:H:351:PRO:HD3	1.89	0.43
1:G:510:ILE:HD13	1:G:526:TRP:NE1	2.34	0.43
1:H:326:LYS:HD2	1:H:328:LEU:HD11	2.00	0.42
1:H:310:LEU:HD23	1:H:429:VAL:HG11	2.01	0.42
1:G:122:ASN:HD21	5:G:707:1PE:H251	1.84	0.42
1:J:155:GLU:O	1:J:158:LYS:HG2	2.19	0.42
1:C:153:VAL:O	1:C:157:LEU:HG	2.19	0.42
1:G:488:THR:HG21	1:G:555:SER:HA	2.01	0.42
5:I:706:1PE:H242	8:I:924:HOH:O	2.19	0.42
1:L:103:TYR:HB3	5:L:706:1PE:H252	2.01	0.42
1:L:292:TYR:O	1:L:296:GLN:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:400:MET:HE2	1:E:404:ALA:HB2	2.01	0.42
1:J:552:LYS:O	1:J:553:ALA:HB3	2.19	0.42
1:E:321:LEU:HD11	1:E:411:TYR:HA	2.01	0.42
1:K:300:ALA:HA	1:K:301:PRO:HD3	1.82	0.42
1:A:357:LEU:HB2	1:A:425:PHE:HB2	2.00	0.42
1:J:300:ALA:HA	1:J:301:PRO:HD3	1.92	0.42
1:J:364:ASP:O	1:J:420:ASN:HA	2.19	0.42
1:B:294:ALA:O	1:B:298:ILE:HG13	2.20	0.42
1:B:342:LEU:HD12	1:C:94:LEU:HD12	2.01	0.42
1:E:214:LEU:HD21	1:E:222:LEU:HD22	2.02	0.42
1:B:181:ASN:ND2	1:B:183:ASN:OD1	2.52	0.42
1:A:114:VAL:HG12	1:A:274:ALA:HB1	2.02	0.42
1:F:207:VAL:HG11	1:F:241:THR:HG22	2.02	0.42
1:F:300:ALA:HA	1:F:301:PRO:HD3	1.86	0.42
1:C:126:GLY:O	1:C:221:LYS:O	2.37	0.42
1:G:340:ALA:HA	1:G:445:ILE:HD12	2.01	0.42
1:G:173:LYS:HD2	1:J:176:TYR:HE1	1.84	0.42
1:J:413:VAL:HG11	1:J:423:ILE:HD12	2.01	0.42
1:C:544:ILE:CD1	1:C:564:GLU:HG3	2.50	0.42
1:I:150:ASP:OD2	1:I:179:ASN:HB2	2.20	0.42
1:F:372:VAL:O	1:F:483:ASP:HA	2.20	0.42
1:H:231:ASP:OD1	1:H:231:ASP:N	2.49	0.42
1:J:483:ASP:OD1	1:J:573:HIS:ND1	2.37	0.42
1:A:178:PHE:CZ	1:D:155:GLU:HG2	2.55	0.41
1:K:544:ILE:HD12	1:K:564:GLU:HG3	2.01	0.41
1:J:551:VAL:HG12	1:J:552:LYS:O	2.20	0.41
1:C:135:PRO:HA	1:C:194:SER:O	2.19	0.41
1:K:158:LYS:HE2	1:K:161:ASN:ND2	2.34	0.41
1:L:150:ASP:OD2	1:L:179:ASN:HB2	2.20	0.41
1:H:488:THR:HG21	1:H:555:SER:HA	2.02	0.41
1:D:300:ALA:HA	1:D:301:PRO:HD3	1.92	0.41
1:E:150:ASP:OD2	1:E:179:ASN:HB2	2.21	0.41
4:C:704:4ZN:O10	4:C:704:4ZN:H20	2.20	0.41
1:D:342:LEU:HA	1:D:342:LEU:HD23	1.89	0.41
1:L:418:PRO:HB3	1:L:601:LEU:HD12	2.03	0.41
1:B:372:VAL:O	1:B:483:ASP:HA	2.20	0.41
1:B:287:TYR:CD2	1:B:594:ARG:HG2	2.56	0.41
1:J:294:ALA:O	1:J:298:ILE:HG13	2.20	0.41
1:J:106:PRO:HD3	8:J:1001:HOH:O	2.20	0.41
1:J:214:LEU:HD11	1:J:222:LEU:HD22	2.02	0.41
1:C:488:THR:HG22	8:C:1002:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:346:LYS:HB3	1:J:437:ASN:O	2.20	0.41
1:H:138:GLU:O	1:H:194:SER:OG	2.39	0.41
1:F:396:MET:SD	1:F:398:PHE:HE2	2.44	0.41
1:J:320:LYS:HB3	5:J:707:1PE:H242	2.02	0.41
1:D:132:VAL:HG11	1:D:144:ILE:HD13	2.02	0.41
1:G:551:VAL:O	1:G:552:LYS:HB2	2.21	0.41
1:B:383:TYR:HE1	1:B:438:SER:HB2	1.85	0.41
1:H:499:TYR:CD1	1:H:523:PRO:HB2	2.55	0.41
1:I:328:LEU:HB2	1:I:354:PHE:HB3	2.02	0.41
1:I:536:THR:HG21	1:I:551:VAL:HG23	2.03	0.41
1:J:321:LEU:CD1	1:J:411:TYR:HA	2.51	0.41
1:K:302:SER:OG	1:K:378:PHE:HB2	2.21	0.41
1:I:400:MET:H	1:I:400:MET:HG3	1.27	0.41
1:J:372:VAL:O	1:J:483:ASP:HA	2.20	0.40
1:L:138:GLU:N	1:L:139:ASN:CA	2.83	0.40
1:F:436:LYS:HB3	1:F:436:LYS:HE2	1.98	0.40
1:D:210:LEU:HD12	1:D:213:MET:HE3	2.02	0.40
1:H:449:ASN:HD21	1:H:451:LYS:HD2	1.86	0.40
1:C:340:ALA:HA	1:C:445:ILE:HD12	2.02	0.40
1:J:341:TYR:CE1	1:J:428:ALA:HB1	2.56	0.40
1:B:235:PHE:O	1:B:238:PHE:HB3	2.20	0.40
1:E:103:TYR:CD2	5:E:705:1PE:H132	2.56	0.40
1:D:364:ASP:O	1:D:420:ASN:HA	2.21	0.40
1:H:203:MET:SD	1:H:238:PHE:HD1	2.45	0.40
1:I:300:ALA:HA	1:I:301:PRO:HD3	1.86	0.40
1:C:300:ALA:HA	1:C:301:PRO:HD3	1.86	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	518/519 (100%)	501 (97%)	16 (3%)	1 (0%)	52	64
1	B	512/519 (99%)	495 (97%)	16 (3%)	1 (0%)	52	64
1	C	515/519 (99%)	499 (97%)	15 (3%)	1 (0%)	52	64
1	D	510/519 (98%)	496 (97%)	13 (2%)	1 (0%)	52	64
1	E	503/519 (97%)	493 (98%)	10 (2%)	0	100	100
1	F	507/519 (98%)	490 (97%)	17 (3%)	0	100	100
1	G	517/519 (100%)	503 (97%)	14 (3%)	0	100	100
1	H	513/519 (99%)	500 (98%)	11 (2%)	2 (0%)	39	48
1	I	515/519 (99%)	505 (98%)	8 (2%)	2 (0%)	39	48
1	J	510/519 (98%)	496 (97%)	12 (2%)	2 (0%)	39	48
1	K	503/519 (97%)	490 (97%)	10 (2%)	3 (1%)	30	36
1	L	507/519 (98%)	491 (97%)	14 (3%)	2 (0%)	39	48
All	All	6130/6228 (98%)	5959 (97%)	156 (2%)	15 (0%)	52	64

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	551	VAL
1	H	138	GLU
1	K	100	PRO
1	K	551	VAL
1	K	552	LYS
1	L	550	SER
1	J	551	VAL
1	L	552	LYS
1	C	126	GLY
1	B	149	ASN
1	J	137	LYS
1	H	254	SER
1	I	137	LYS
1	I	261	MET
1	D	551	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	423/447 (95%)	417 (99%)	6 (1%)	74	86
1	B	407/447 (91%)	403 (99%)	4 (1%)	82	91
1	C	418/447 (94%)	406 (97%)	12 (3%)	50	66
1	D	413/447 (92%)	405 (98%)	8 (2%)	65	81
1	E	413/447 (92%)	410 (99%)	3 (1%)	88	95
1	F	402/447 (90%)	391 (97%)	11 (3%)	52	70
1	G	422/447 (94%)	415 (98%)	7 (2%)	68	83
1	H	406/447 (91%)	397 (98%)	9 (2%)	60	77
1	I	420/447 (94%)	414 (99%)	6 (1%)	74	86
1	J	414/447 (93%)	408 (99%)	6 (1%)	74	86
1	K	410/447 (92%)	406 (99%)	4 (1%)	82	91
1	L	400/447 (90%)	394 (98%)	6 (2%)	72	85
All	All	4948/5364 (92%)	4866 (98%)	82 (2%)	68	83

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	288	TYR
1	A	398	PHE
1	A	400	MET
1	A	436	LYS
1	A	439	TYR
1	A	554	SER
1	B	288	TYR
1	B	398	PHE
1	B	439	TYR
1	B	549	SER
1	C	86	SER
1	C	185	VAL
1	C	272	ASN
1	C	276	THR
1	C	295	SER
1	C	398	PHE
1	C	400	MET
1	C	439	TYR
1	C	483	ASP

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Mol	Chain	Res	Type
1	C	549	SER
1	C	550	SER
1	C	554	SER
1	D	200	GLU
1	D	250	GLU
1	D	262	GLU
1	D	288	TYR
1	D	398	PHE
1	D	439	TYR
1	D	483	ASP
1	D	568	ASN
1	E	398	PHE
1	E	400	MET
1	E	439	TYR
1	F	167	VAL
1	F	169	LEU
1	F	200	GLU
1	F	215	HIS
1	F	219	LEU
1	F	248	THR
1	F	288	TYR
1	F	361	SER
1	F	398	PHE
1	F	439	TYR
1	F	494	SER
1	G	200	GLU
1	G	288	TYR
1	G	398	PHE
1	G	400	MET
1	G	439	TYR
1	G	554	SER
1	G	568	ASN
1	H	139	ASN
1	H	142	VAL
1	H	288	TYR
1	H	328	LEU
1	H	398	PHE
1	H	439	TYR
1	H	483	ASP
1	H	549	SER
1	H	554	SER
1	I	86	SER

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Mol	Chain	Res	Type
1	I	288	TYR
1	I	398	PHE
1	I	400	MET
1	I	439	TYR
1	I	483	ASP
1	J	200	GLU
1	J	288	TYR
1	J	398	PHE
1	J	439	TYR
1	J	511	ASN
1	J	567	GLN
1	K	230	VAL
1	K	395	LEU
1	K	398	PHE
1	K	439	TYR
1	L	200	GLU
1	L	288	TYR
1	L	398	PHE
1	L	435	SER
1	L	439	TYR
1	L	568	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	260	ASN
1	B	181	ASN
1	G	122	ASN
1	G	149	ASN
1	H	139	ASN
1	J	181	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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



## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 102 ligands modelled in this entry, 24 are monoatomic - leaving 78 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	CO3	A	701	-	0,3,3	0.00	-	0,3,3	0.00	-
4	4ZN	A	704	3	10,16,20	0.40	0	12,22,28	1.52	2 (16%)
5	1PE	A	705	-	8,8,15	0.76	0	7,7,14	0.33	0
5	1PE	A	706	-	11,11,15	0.80	0	10,10,14	0.34	0
6	GOL	A	707	-	5,5,5	0.44	0	5,5,5	0.22	0
7	SO4	A	708	-	4,4,4	0.12	0	6,6,6	0.16	0
7	SO4	A	709	-	4,4,4	0.10	0	6,6,6	0.17	0
7	SO4	A	710	-	4,4,4	0.12	0	6,6,6	0.28	0
7	SO4	A	711	-	4,4,4	0.12	0	6,6,6	0.21	0
7	SO4	A	712	-	4,4,4	0.24	0	6,6,6	0.53	0
2	CO3	B	701	-	0,3,3	0.00	-	0,3,3	0.00	-
4	4ZN	B	704	3	10,16,20	0.77	0	12,22,28	2.65	5 (41%)
5	1PE	B	705	-	9,9,15	0.71	0	8,8,14	0.38	0
5	1PE	B	706	-	9,9,15	0.73	0	8,8,14	0.46	0
7	SO4	B	707	-	4,4,4	0.22	0	6,6,6	0.31	0
2	CO3	C	701	-	0,3,3	0.00	-	0,3,3	0.00	-
4	4ZN	C	704	3	10,16,20	1.47	1 (10%)	12,22,28	1.08	1 (8%)
5	1PE	C	705	-	12,12,15	0.81	0	11,11,14	0.55	0
5	1PE	C	706	-	8,8,15	0.79	0	7,7,14	0.30	0
7	SO4	C	707	-	4,4,4	0.16	0	6,6,6	0.11	0
7	SO4	C	708	-	4,4,4	0.10	0	6,6,6	0.36	0
7	SO4	C	709	-	4,4,4	0.19	0	6,6,6	0.40	0
7	SO4	C	710	-	4,4,4	0.21	0	6,6,6	0.24	0
7	SO4	C	711	-	4,4,4	0.23	0	6,6,6	0.39	0
2	CO3	D	701	-	0,3,3	0.00	-	0,3,3	0.00	-
4	4ZN	D	704	3	13,20,20	1.42	2 (15%)	18,28,28	2.51	5 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	1PE	D	705	-	9,9,15	0.83	0	8,8,14	0.46	0
5	1PE	D	706	-	9,9,15	0.77	0	8,8,14	0.34	0
7	SO4	D	707	-	4,4,4	0.19	0	6,6,6	0.20	0
2	CO3	E	701	-	0,3,3	0.00	-	0,3,3	0.00	-
4	4ZN	E	704	3	13,20,20	0.72	1 (7%)	18,28,28	2.07	6 (33%)
5	1PE	E	705	-	11,11,15	0.84	0	10,10,14	0.39	0
5	1PE	E	706	-	11,11,15	0.72	0	10,10,14	0.32	0
7	SO4	E	707	-	4,4,4	0.20	0	6,6,6	0.14	0
7	SO4	E	708	-	4,4,4	0.22	0	6,6,6	0.25	0
7	SO4	E	709	-	4,4,4	0.13	0	6,6,6	0.09	0
2	CO3	F	701	-	0,3,3	0.00	-	0,3,3	0.00	-
4	4ZN	F	704	3	10,16,20	0.56	0	12,22,28	1.69	3 (25%)
5	1PE	F	705	-	9,9,15	0.70	0	8,8,14	0.40	0
7	SO4	F	706	-	4,4,4	0.17	0	6,6,6	0.20	0
7	SO4	F	707	-	4,4,4	0.10	0	6,6,6	0.09	0
2	CO3	G	701	-	0,3,3	0.00	-	0,3,3	0.00	-
4	4ZN	G	704	3	10,16,20	0.47	0	12,22,28	1.89	3 (25%)
5	1PE	G	705	-	8,8,15	0.71	0	7,7,14	0.34	0
5	1PE	G	706	-	5,5,15	0.61	0	4,4,14	0.59	0
5	1PE	G	707	-	5,5,15	0.69	0	4,4,14	0.42	0
7	SO4	G	708	-	4,4,4	0.18	0	6,6,6	0.19	0
7	SO4	G	709	-	4,4,4	0.18	0	6,6,6	0.33	0
7	SO4	G	710	-	4,4,4	0.12	0	6,6,6	0.19	0
7	SO4	G	711	-	4,4,4	0.29	0	6,6,6	0.49	0
2	CO3	H	701	-	0,3,3	0.00	-	0,3,3	0.00	-
4	4ZN	H	704	3	10,16,20	1.73	2 (20%)	12,22,28	1.40	2 (16%)
5	1PE	H	705	-	9,9,15	0.77	0	8,8,14	0.27	0
5	1PE	H	706	-	9,9,15	0.76	0	8,8,14	0.20	0
2	CO3	I	701	-	0,3,3	0.00	-	0,3,3	0.00	-
4	4ZN	I	704	3	7,12,20	0.69	0	10,17,28	0.77	0
5	1PE	I	705	-	11,11,15	0.77	0	10,10,14	0.39	0
5	1PE	I	706	-	10,10,15	0.72	0	9,9,14	0.45	0
7	SO4	I	707	-	4,4,4	0.18	0	6,6,6	0.17	0
7	SO4	I	708	-	4,4,4	0.12	0	6,6,6	0.08	0
2	CO3	J	701	-	0,3,3	0.00	-	0,3,3	0.00	-
4	4ZN	J	704	3	10,16,20	1.44	1 (10%)	12,22,28	1.27	1 (8%)
5	1PE	J	705	-	10,10,15	0.70	0	9,9,14	0.41	0
5	1PE	J	706	-	10,10,15	0.73	0	9,9,14	0.48	0
5	1PE	J	707	-	9,9,15	0.62	0	8,8,14	0.34	0
7	SO4	J	708	-	4,4,4	0.25	0	6,6,6	0.21	0
7	SO4	J	709	-	4,4,4	0.40	0	6,6,6	0.17	0
2	CO3	K	701	-	0,3,3	0.00	-	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	4ZN	K	704	3	11,14,20	0.80	1 (9%)	14,19,28	1.82	2 (14%)
5	1PE	K	705	-	11,11,15	0.73	0	10,10,14	0.26	0
5	1PE	K	706	-	11,11,15	0.75	0	10,10,14	0.44	0
7	SO4	K	707	-	4,4,4	0.23	0	6,6,6	0.10	0
7	SO4	K	708	-	4,4,4	0.08	0	6,6,6	0.28	0
2	CO3	L	701	-	0,3,3	0.00	-	0,3,3	0.00	-
4	4ZN	L	704	3	10,16,20	0.53	0	12,22,28	1.49	1 (8%)
5	1PE	L	705	-	6,6,15	0.72	0	5,5,14	0.39	0
5	1PE	L	706	-	9,9,15	0.63	0	8,8,14	0.43	0
7	SO4	L	707	-	4,4,4	0.24	0	6,6,6	0.18	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CO3	A	701	-	-	0/0/0/0	0/0/0/0
4	4ZN	A	704	3	-	0/9/16/23	0/1/1/1
5	1PE	A	705	-	-	0/6/6/13	0/0/0/0
5	1PE	A	706	-	-	0/9/9/13	0/0/0/0
6	GOL	A	707	-	-	0/4/4/4	0/0/0/0
7	SO4	A	708	-	-	0/0/0/0	0/0/0/0
7	SO4	A	709	-	-	0/0/0/0	0/0/0/0
7	SO4	A	710	-	-	0/0/0/0	0/0/0/0
7	SO4	A	711	-	-	0/0/0/0	0/0/0/0
7	SO4	A	712	-	-	0/0/0/0	0/0/0/0
2	CO3	B	701	-	-	0/0/0/0	0/0/0/0
4	4ZN	B	704	3	-	0/9/16/23	0/1/1/1
5	1PE	B	705	-	-	0/7/7/13	0/0/0/0
5	1PE	B	706	-	-	0/7/7/13	0/0/0/0
7	SO4	B	707	-	-	0/0/0/0	0/0/0/0
2	CO3	C	701	-	-	0/0/0/0	0/0/0/0
4	4ZN	C	704	3	-	0/9/16/23	0/1/1/1
5	1PE	C	705	-	-	0/10/10/13	0/0/0/0
5	1PE	C	706	-	-	0/6/6/13	0/0/0/0
7	SO4	C	707	-	-	0/0/0/0	0/0/0/0
7	SO4	C	708	-	-	0/0/0/0	0/0/0/0
7	SO4	C	709	-	-	0/0/0/0	0/0/0/0
7	SO4	C	710	-	-	0/0/0/0	0/0/0/0
7	SO4	C	711	-	-	0/0/0/0	0/0/0/0
2	CO3	D	701	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	4ZN	D	704	3	-	0/13/23/23	0/1/1/1
5	1PE	D	705	-	-	0/7/7/13	0/0/0/0
5	1PE	D	706	-	-	0/7/7/13	0/0/0/0
7	SO4	D	707	-	-	0/0/0/0	0/0/0/0
2	CO3	E	701	-	-	0/0/0/0	0/0/0/0
4	4ZN	E	704	3	-	0/13/23/23	0/1/1/1
5	1PE	E	705	-	-	0/9/9/13	0/0/0/0
5	1PE	E	706	-	-	0/9/9/13	0/0/0/0
7	SO4	E	707	-	-	0/0/0/0	0/0/0/0
7	SO4	E	708	-	-	0/0/0/0	0/0/0/0
7	SO4	E	709	-	-	0/0/0/0	0/0/0/0
2	CO3	F	701	-	-	0/0/0/0	0/0/0/0
4	4ZN	F	704	3	-	0/9/16/23	0/1/1/1
5	1PE	F	705	-	-	0/7/7/13	0/0/0/0
7	SO4	F	706	-	-	0/0/0/0	0/0/0/0
7	SO4	F	707	-	-	0/0/0/0	0/0/0/0
2	CO3	G	701	-	-	0/0/0/0	0/0/0/0
4	4ZN	G	704	3	-	0/9/16/23	0/1/1/1
5	1PE	G	705	-	-	0/6/6/13	0/0/0/0
5	1PE	G	706	-	-	0/3/3/13	0/0/0/0
5	1PE	G	707	-	-	0/3/3/13	0/0/0/0
7	SO4	G	708	-	-	0/0/0/0	0/0/0/0
7	SO4	G	709	-	-	0/0/0/0	0/0/0/0
7	SO4	G	710	-	-	0/0/0/0	0/0/0/0
7	SO4	G	711	-	-	0/0/0/0	0/0/0/0
2	CO3	H	701	-	-	0/0/0/0	0/0/0/0
4	4ZN	H	704	3	-	0/9/16/23	0/1/1/1
5	1PE	H	705	-	-	0/7/7/13	0/0/0/0
5	1PE	H	706	-	-	0/7/7/13	0/0/0/0
2	CO3	I	701	-	-	0/0/0/0	0/0/0/0
4	4ZN	I	704	3	-	0/5/10/23	0/1/1/1
5	1PE	I	705	-	-	0/9/9/13	0/0/0/0
5	1PE	I	706	-	-	0/8/8/13	0/0/0/0
7	SO4	I	707	-	-	0/0/0/0	0/0/0/0
7	SO4	I	708	-	-	0/0/0/0	0/0/0/0
2	CO3	J	701	-	-	0/0/0/0	0/0/0/0
4	4ZN	J	704	3	-	0/9/16/23	0/1/1/1
5	1PE	J	705	-	-	0/8/8/13	0/0/0/0
5	1PE	J	706	-	-	0/8/8/13	0/0/0/0
5	1PE	J	707	-	-	0/7/7/13	0/0/0/0
7	SO4	J	708	-	-	0/0/0/0	0/0/0/0
7	SO4	J	709	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CO3	K	701	-	-	0/0/0/0	0/0/0/0
4	4ZN	K	704	3	-	0/9/14/23	0/1/1/1
5	1PE	K	705	-	-	0/9/9/13	0/0/0/0
5	1PE	K	706	-	-	0/9/9/13	0/0/0/0
7	SO4	K	707	-	-	0/0/0/0	0/0/0/0
7	SO4	K	708	-	-	0/0/0/0	0/0/0/0
2	CO3	L	701	-	-	0/0/0/0	0/0/0/0
4	4ZN	L	704	3	-	0/9/16/23	0/1/1/1
5	1PE	L	705	-	-	0/4/4/13	0/0/0/0
5	1PE	L	706	-	-	0/7/7/13	0/0/0/0
7	SO4	L	707	-	-	0/0/0/0	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	704	4ZN	P08-C07	2.13	1.81	1.79
4	K	704	4ZN	P08-C07	2.21	1.81	1.79
4	H	704	4ZN	P08-C07	2.61	1.82	1.79
4	D	704	4ZN	P08-C07	2.86	1.82	1.79
4	D	704	4ZN	P08-O10	4.16	1.57	1.49
4	C	704	4ZN	P08-O10	4.28	1.58	1.49
4	J	704	4ZN	P08-O10	4.45	1.58	1.49
4	H	704	4ZN	P08-O10	4.67	1.58	1.49

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	704	4ZN	O09-P08-O10	-6.55	102.90	114.00
4	B	704	4ZN	O09-P08-O10	-6.48	103.02	114.00
4	K	704	4ZN	O09-P08-O10	-4.92	105.67	114.00
4	G	704	4ZN	O09-P08-O10	-4.27	106.76	114.00
4	L	704	4ZN	O09-P08-O10	-4.01	107.20	114.00
4	A	704	4ZN	O09-P08-O10	-3.64	107.83	114.00
4	H	704	4ZN	O09-P08-O10	-3.61	107.88	114.00
4	B	704	4ZN	O10-P08-C11	-3.52	104.65	111.48
4	E	704	4ZN	O09-P08-O10	-3.45	108.15	114.00
4	F	704	4ZN	O09-P08-O10	-3.36	108.30	114.00
4	E	704	4ZN	O10-P08-C11	-3.14	105.38	111.48
4	G	704	4ZN	O10-P08-C11	-3.07	105.52	111.48
4	D	704	4ZN	C13-C11-N12	-3.01	104.80	112.92
4	D	704	4ZN	C18-C13-C11	-3.00	117.83	120.70
4	J	704	4ZN	O09-P08-O10	-2.99	108.93	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	704	4ZN	O09-P08-O10	-2.95	109.01	114.00
4	B	704	4ZN	C18-C13-C11	-2.90	117.92	120.70
4	A	704	4ZN	O10-P08-C11	-2.76	106.12	111.48
4	E	704	4ZN	C13-C11-N12	-2.62	105.85	112.92
4	K	704	4ZN	O10-P08-C11	-2.50	106.62	111.48
4	E	704	4ZN	C18-C13-C11	-2.24	118.56	120.70
4	H	704	4ZN	C13-C11-N12	-2.22	106.92	112.92
4	F	704	4ZN	C13-C11-N12	-2.18	107.04	112.92
4	B	704	4ZN	C14-C13-C11	2.28	122.89	120.70
4	G	704	4ZN	P08-C11-C13	2.88	116.73	111.73
4	D	704	4ZN	C06-C05-C03	3.05	122.74	115.85
4	F	704	4ZN	P08-C11-C13	3.14	117.18	111.73
4	E	704	4ZN	P08-C11-C13	3.78	118.30	111.73
4	B	704	4ZN	P08-C11-C13	3.88	118.47	111.73
4	E	704	4ZN	C06-C05-C03	4.21	125.35	115.85
4	D	704	4ZN	P08-C11-C13	5.31	120.95	111.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

32 monomers are involved in 59 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	704	4ZN	2	0
7	A	712	SO4	2	0
4	B	704	4ZN	3	0
5	B	706	1PE	3	0
4	C	704	4ZN	1	0
5	C	706	1PE	1	0
7	C	708	SO4	1	0
7	C	711	SO4	1	0
4	D	704	4ZN	3	0
5	D	705	1PE	2	0
7	D	707	SO4	1	0
4	E	704	4ZN	2	0
5	E	705	1PE	1	0
5	E	706	1PE	1	0
7	E	707	SO4	1	0
5	G	705	1PE	1	0
5	G	706	1PE	2	0
5	G	707	1PE	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	711	SO4	2	0
4	H	704	4ZN	1	0
5	H	705	1PE	1	0
5	I	705	1PE	1	0
5	I	706	1PE	1	0
4	J	704	4ZN	2	0
5	J	705	1PE	4	0
5	J	706	1PE	5	0
5	J	707	1PE	3	0
4	K	704	4ZN	1	0
5	K	706	1PE	2	0
4	L	704	4ZN	1	0
5	L	705	1PE	5	0
5	L	706	1PE	1	0

## 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	519/519 (100%)	3.49	451 (86%) <b>0</b> <b>0</b>	14, 23, 41, 61	3 (0%)
1	B	516/519 (99%)	3.62	434 (84%) <b>0</b> <b>0</b>	13, 25, 56, 73	5 (0%)
1	C	517/519 (99%)	3.28	451 (87%) <b>0</b> <b>0</b>	13, 23, 43, 60	3 (0%)
1	D	514/519 (99%)	2.97	401 (78%) <b>0</b> <b>0</b>	14, 23, 38, 58	1 (0%)
1	E	509/519 (98%)	3.19	424 (83%) <b>0</b> <b>0</b>	13, 22, 35, 48	2 (0%)
1	F	511/519 (98%)	3.47	426 (83%) <b>0</b> <b>0</b>	16, 26, 54, 71	9 (1%)
1	G	519/519 (100%)	3.39	446 (85%) <b>0</b> <b>0</b>	14, 23, 40, 55	5 (0%)
1	H	517/519 (99%)	3.67	447 (86%) <b>0</b> <b>0</b>	14, 27, 58, 73	5 (0%)
1	I	517/519 (99%)	3.32	438 (84%) <b>0</b> <b>0</b>	13, 25, 46, 63	5 (0%)
1	J	514/519 (99%)	3.09	411 (79%) <b>0</b> <b>0</b>	13, 23, 39, 55	6 (1%)
1	K	509/519 (98%)	3.22	428 (84%) <b>0</b> <b>0</b>	15, 23, 37, 62	3 (0%)
1	L	511/519 (98%)	3.47	424 (82%) <b>0</b> <b>0</b>	15, 25, 52, 62	6 (1%)
All	All	6173/6228 (99%)	3.35	5181 (83%) <b>0</b> <b>0</b>	13, 24, 49, 73	53 (0%)

All (5181) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	136	GLY	13.2
1	J	603	ASP	12.6
1	F	121	CYS	12.0
1	L	363	GLY	12.0
1	H	261	MET	11.4
1	D	85	ALA	10.9
1	B	272	ASN	10.9
1	F	138	GLU	10.9
1	J	136	GLY	10.8
1	H	255	THR	10.8
1	L	197	ASP	10.7

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Mol	Chain	Res	Type	RSRZ
1	B	121	CYS	10.2
1	A	363	GLY	10.0
1	H	135	PRO	9.6
1	L	138	GLU	9.6
1	L	153	VAL	9.5
1	B	202	ASP	9.3
1	F	197	ASP	9.3
1	L	119	GLY	9.3
1	B	150	ASP	9.2
1	L	147	LYS	9.2
1	D	136	GLY	9.0
1	G	551	VAL	9.0
1	E	549	SER	9.0
1	B	600	VAL	8.9
1	I	230	VAL	8.8
1	B	157	LEU	8.7
1	L	494	SER	8.7
1	H	144	ILE	8.7
1	B	228	ILE	8.7
1	B	261	MET	8.7
1	D	603	ASP	8.6
1	F	267	LEU	8.5
1	H	603	ASP	8.5
1	H	597	THR	8.5
1	J	363	GLY	8.5
1	F	549	SER	8.5
1	H	257	LYS	8.5
1	F	178	PHE	8.4
1	B	118	LYS	8.4
1	F	88	VAL	8.4
1	H	189	TYR	8.4
1	I	576	ILE	8.4
1	H	202	ASP	8.3
1	C	136	GLY	8.3
1	K	99	ILE	8.2
1	H	260	ASN	8.2
1	B	143	LYS	8.1
1	F	180	ASP	8.1
1	B	144	ILE	8.1
1	I	121	CYS	8.1
1	L	364	ASP	8.0
1	A	362	LYS	8.0

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Mol	Chain	Res	Type	RSRZ
1	A	603	ASP	8.0
1	B	161	ASN	7.9
1	C	134	ASN	7.9
1	A	550	SER	7.9
1	L	134	ASN	7.8
1	H	165	PHE	7.8
1	L	159	ASP	7.8
1	D	196	ALA	7.8
1	F	159	ASP	7.8
1	H	276	THR	7.8
1	B	123	VAL	7.7
1	G	550	SER	7.7
1	F	179	ASN	7.7
1	K	576	ILE	7.7
1	A	600	VAL	7.7
1	B	403	CYS	7.6
1	B	271	ILE	7.6
1	I	510	ILE	7.6
1	I	117	ILE	7.6
1	E	576	ILE	7.6
1	D	198	LEU	7.6
1	F	364	ASP	7.6
1	B	132	VAL	7.6
1	B	165	PHE	7.6
1	C	163	GLU	7.6
1	B	255	THR	7.5
1	H	217	ASN	7.5
1	A	85	ALA	7.5
1	H	225	VAL	7.4
1	E	596	LEU	7.4
1	B	149	ASN	7.4
1	C	365	VAL	7.4
1	I	565	PHE	7.4
1	L	144	ILE	7.3
1	K	558	ALA	7.3
1	G	557	VAL	7.3
1	H	117	ILE	7.3
1	J	300	ALA	7.3
1	H	185	VAL	7.3
1	F	141	PRO	7.3
1	B	549	SER	7.3
1	J	600	VAL	7.3

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Mol	Chain	Res	Type	RSRZ
1	H	239	LEU	7.3
1	H	159	ASP	7.3
1	C	88	VAL	7.2
1	J	178	PHE	7.2
1	B	195	VAL	7.2
1	D	547	ILE	7.2
1	B	557	VAL	7.2
1	F	145	SER	7.2
1	H	157	LEU	7.2
1	J	123	VAL	7.2
1	B	229	ASN	7.2
1	H	155	GLU	7.2
1	H	549	SER	7.2
1	J	184	SER	7.2
1	B	446	THR	7.2
1	K	551	VAL	7.1
1	I	140	GLY	7.1
1	L	135	PRO	7.1
1	F	434	VAL	7.1
1	L	148	VAL	7.1
1	B	192	CYS	7.1
1	E	395	LEU	7.1
1	F	185	VAL	7.1
1	J	196	ALA	7.1
1	K	419	GLU	7.1
1	A	256	ASP	7.1
1	I	135	PRO	7.1
1	B	131	LEU	7.1
1	A	398	PHE	7.1
1	F	377	THR	7.0
1	F	579	VAL	7.0
1	A	295	SER	7.0
1	B	136	GLY	7.0
1	C	194	SER	7.0
1	L	161	ASN	7.0
1	B	363	GLY	7.0
1	A	130	PHE	7.0
1	F	144	ILE	7.0
1	H	234	LEU	7.0
1	H	333	LEU	7.0
1	F	142	VAL	7.0
1	B	122	ASN	6.9

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Mol	Chain	Res	Type	RSRZ
1	G	267	LEU	6.9
1	H	141	PRO	6.9
1	G	261	MET	6.9
1	F	123	VAL	6.9
1	E	294	ALA	6.9
1	H	143	LYS	6.9
1	H	154	SER	6.9
1	K	305	CYS	6.8
1	L	121	CYS	6.8
1	B	197	ASP	6.8
1	E	391	SER	6.8
1	A	260	ASN	6.8
1	H	134	ASN	6.8
1	H	275	ASP	6.8
1	K	406	VAL	6.8
1	B	548	SER	6.8
1	L	177	MET	6.8
1	L	550	SER	6.8
1	E	148	VAL	6.8
1	H	122	ASN	6.8
1	L	434	VAL	6.8
1	L	487	LEU	6.7
1	H	180	ASP	6.7
1	L	322	ASN	6.7
1	I	93	SER	6.7
1	B	153	VAL	6.7
1	B	269	VAL	6.7
1	H	486	THR	6.7
1	B	156	PHE	6.7
1	K	210	LEU	6.7
1	L	183	ASN	6.7
1	I	292	TYR	6.7
1	F	117	ILE	6.7
1	F	122	ASN	6.7
1	F	106	PRO	6.7
1	H	132	VAL	6.7
1	F	600	VAL	6.6
1	L	603	ASP	6.6
1	C	403	CYS	6.6
1	G	600	VAL	6.6
1	C	602	ASN	6.6
1	L	178	PHE	6.6

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Mol	Chain	Res	Type	RSRZ
1	E	466	LEU	6.6
1	J	194	SER	6.6
1	A	305	CYS	6.6
1	G	286	VAL	6.6
1	J	183	ASN	6.6
1	H	201	ALA	6.6
1	C	132	VAL	6.5
1	L	230	VAL	6.5
1	L	156	PHE	6.5
1	C	310	LEU	6.5
1	I	294	ALA	6.5
1	L	179	ASN	6.5
1	A	576	ILE	6.5
1	H	130	PHE	6.5
1	B	234	LEU	6.5
1	B	133	ASN	6.5
1	E	484	ILE	6.5
1	B	277	TYR	6.5
1	I	407	LEU	6.5
1	H	365	VAL	6.5
1	I	387	ALA	6.5
1	K	509	LEU	6.5
1	B	301	PRO	6.5
1	F	268	GLY	6.5
1	J	471	VAL	6.5
1	B	556	ILE	6.4
1	C	407	LEU	6.4
1	G	342	LEU	6.4
1	B	274	ALA	6.4
1	E	372	VAL	6.4
1	G	562	LEU	6.4
1	G	85	ALA	6.4
1	B	148	VAL	6.4
1	H	123	VAL	6.4
1	F	114	VAL	6.4
1	H	137	LYS	6.4
1	F	157	LEU	6.4
1	I	200	GLU	6.4
1	L	145	SER	6.4
1	C	576	ILE	6.4
1	A	277	TYR	6.4
1	F	272	ASN	6.4

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Mol	Chain	Res	Type	RSRZ
1	L	485	ALA	6.4
1	G	365	VAL	6.4
1	H	423	ILE	6.4
1	J	148	VAL	6.4
1	A	194	SER	6.4
1	E	551	VAL	6.3
1	I	466	LEU	6.3
1	A	119	GLY	6.3
1	C	297	LEU	6.3
1	C	180	ASP	6.3
1	I	138	GLU	6.3
1	A	99	ILE	6.3
1	D	576	ILE	6.3
1	F	110	ILE	6.3
1	K	385	LEU	6.3
1	L	234	LEU	6.3
1	G	585	ALA	6.3
1	E	376	ILE	6.3
1	I	542	ALA	6.3
1	A	572	ALA	6.3
1	F	270	TYR	6.2
1	G	211	VAL	6.2
1	K	510	ILE	6.2
1	B	145	SER	6.2
1	B	184	SER	6.2
1	H	230	VAL	6.2
1	E	409	CYS	6.2
1	E	420	ASN	6.2
1	J	396	MET	6.2
1	B	199	SER	6.2
1	G	404	ALA	6.2
1	F	342	LEU	6.2
1	C	230	VAL	6.2
1	G	178	PHE	6.2
1	H	138	GLU	6.2
1	A	294	ALA	6.2
1	F	183	ASN	6.2
1	A	487	LEU	6.2
1	F	487	LEU	6.2
1	F	153	VAL	6.2
1	L	410	ALA	6.2
1	G	549	SER	6.2

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Mol	Chain	Res	Type	RSRZ
1	A	485	ALA	6.2
1	H	569	THR	6.2
1	I	144	ILE	6.2
1	G	104	ASN	6.1
1	B	135	PRO	6.1
1	G	363	GLY	6.1
1	H	223	THR	6.1
1	B	162	MET	6.1
1	B	154	SER	6.1
1	B	134	ASN	6.1
1	K	395	LEU	6.1
1	G	246	TYR	6.1
1	B	294	ALA	6.1
1	H	269	VAL	6.1
1	L	155	GLU	6.1
1	H	150	ASP	6.1
1	A	526	TRP	6.1
1	D	426	LEU	6.1
1	G	537	LEU	6.1
1	H	409	CYS	6.1
1	I	579	VAL	6.1
1	L	165	PHE	6.1
1	F	446	THR	6.1
1	F	135	PRO	6.1
1	D	537	LEU	6.1
1	C	211	VAL	6.1
1	C	406	VAL	6.1
1	A	159	ASP	6.0
1	I	146	SER	6.0
1	F	150	ASP	6.0
1	F	398	PHE	6.0
1	I	214	LEU	6.0
1	K	595	LEU	6.0
1	F	151	LYS	6.0
1	I	194	SER	6.0
1	H	187	VAL	6.0
1	L	452	THR	6.0
1	B	416	LEU	6.0
1	A	117	ILE	6.0
1	B	226	PHE	6.0
1	G	289	PHE	6.0
1	G	398	PHE	6.0

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Mol	Chain	Res	Type	RSRZ
1	A	310	LEU	6.0
1	H	145	SER	6.0
1	K	196	ALA	6.0
1	K	410	ALA	6.0
1	L	99	ILE	6.0
1	A	557	VAL	6.0
1	J	406	VAL	6.0
1	J	161	ASN	6.0
1	C	117	ILE	6.0
1	K	364	ASP	6.0
1	E	289	PHE	6.0
1	F	601	LEU	6.0
1	C	363	GLY	5.9
1	J	576	ILE	5.9
1	L	229	ASN	5.9
1	F	577	ALA	5.9
1	G	467	ALA	5.9
1	B	127	LEU	5.9
1	I	272	ASN	5.9
1	C	551	VAL	5.9
1	J	269	VAL	5.9
1	B	146	SER	5.9
1	I	385	LEU	5.9
1	L	323	LEU	5.9
1	D	305	CYS	5.9
1	B	166	ASN	5.9
1	F	155	GLU	5.9
1	F	447	ALA	5.9
1	K	400	MET	5.9
1	H	156	PHE	5.9
1	C	127	LEU	5.9
1	J	298	ILE	5.9
1	K	128	THR	5.9
1	F	148	VAL	5.9
1	E	274	ALA	5.9
1	E	490	ALA	5.9
1	E	421	VAL	5.8
1	I	153	VAL	5.8
1	L	142	VAL	5.8
1	G	242	LEU	5.8
1	L	239	LEU	5.8
1	L	336	LEU	5.8

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Mol	Chain	Res	Type	RSRZ
1	A	110	ILE	5.8
1	C	144	ILE	5.8
1	L	122	ASN	5.8
1	K	376	ILE	5.8
1	H	178	PHE	5.8
1	H	254	SER	5.8
1	A	242	LEU	5.8
1	L	511	ASN	5.8
1	H	146	SER	5.8
1	E	601	LEU	5.8
1	I	202	ASP	5.8
1	F	229	ASN	5.8
1	A	281	VAL	5.8
1	K	185	VAL	5.8
1	L	492	LEU	5.8
1	L	176	TYR	5.8
1	F	376	ILE	5.8
1	J	547	ILE	5.8
1	E	396	MET	5.8
1	H	392	MET	5.8
1	B	93	SER	5.8
1	H	88	VAL	5.8
1	H	128	THR	5.7
1	H	476	LEU	5.7
1	L	544	ILE	5.7
1	I	469	ALA	5.7
1	L	254	SER	5.7
1	L	180	ASP	5.7
1	D	389	PRO	5.7
1	F	492	LEU	5.7
1	H	273	ASN	5.7
1	H	317	LEU	5.7
1	H	232	LYS	5.7
1	B	315	VAL	5.7
1	F	230	VAL	5.7
1	J	308	VAL	5.7
1	B	276	THR	5.7
1	H	198	LEU	5.7
1	A	318	ALA	5.7
1	E	547	ILE	5.7
1	I	114	VAL	5.7
1	B	476	LEU	5.7

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Mol	Chain	Res	Type	RSRZ
1	B	119	GLY	5.7
1	A	455	VAL	5.7
1	L	141	PRO	5.7
1	H	238	PHE	5.7
1	B	322	ASN	5.7
1	I	260	ASN	5.7
1	K	500	ALA	5.7
1	I	162	MET	5.7
1	E	600	VAL	5.7
1	A	255	THR	5.7
1	A	222	LEU	5.7
1	A	601	LEU	5.7
1	C	93	SER	5.7
1	H	136	GLY	5.7
1	H	196	ALA	5.6
1	B	270	TYR	5.6
1	F	211	VAL	5.6
1	K	365	VAL	5.6
1	F	184	SER	5.6
1	B	336	LEU	5.6
1	B	385	LEU	5.6
1	E	410	ALA	5.6
1	I	550	SER	5.6
1	J	315	VAL	5.6
1	J	279	GLU	5.6
1	D	219	LEU	5.6
1	H	318	ALA	5.6
1	A	444	ILE	5.6
1	A	311	SER	5.6
1	G	343	SER	5.6
1	K	375	GLY	5.6
1	A	406	VAL	5.6
1	E	308	VAL	5.6
1	A	267	LEU	5.6
1	K	466	LEU	5.6
1	K	601	LEU	5.6
1	J	228	ILE	5.6
1	H	121	CYS	5.6
1	K	560	LEU	5.6
1	D	362	LYS	5.6
1	H	158	LYS	5.6
1	B	141	PRO	5.6

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Mol	Chain	Res	Type	RSRZ
1	J	122	ASN	5.6
1	B	185	VAL	5.6
1	F	478	VAL	5.6
1	A	214	LEU	5.6
1	B	409	CYS	5.6
1	L	150	ASP	5.6
1	L	88	VAL	5.5
1	A	395	LEU	5.5
1	L	198	LEU	5.5
1	B	196	ALA	5.5
1	H	192	CYS	5.5
1	J	388	ALA	5.5
1	A	583	PHE	5.5
1	A	536	THR	5.5
1	I	393	ILE	5.5
1	A	207	VAL	5.5
1	A	259	VAL	5.5
1	C	579	VAL	5.5
1	D	455	VAL	5.5
1	F	441	PRO	5.5
1	G	317	LEU	5.5
1	H	416	LEU	5.5
1	C	145	SER	5.5
1	H	175	PHE	5.5
1	H	396	MET	5.5
1	G	141	PRO	5.5
1	A	541	TYR	5.5
1	F	254	SER	5.5
1	B	181	ASN	5.5
1	F	181	ASN	5.5
1	F	484	ILE	5.5
1	L	216	ASP	5.5
1	A	593	VAL	5.5
1	D	195	VAL	5.5
1	I	209	SER	5.5
1	C	553	ALA	5.5
1	L	210	LEU	5.5
1	D	122	ASN	5.5
1	E	229	ASN	5.5
1	F	149	ASN	5.5
1	J	121	CYS	5.5
1	B	579	VAL	5.5

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Mol	Chain	Res	Type	RSRZ
1	H	151	LYS	5.5
1	D	94	LEU	5.5
1	G	243	PHE	5.5
1	A	375	GLY	5.5
1	C	581	TRP	5.5
1	A	544	ILE	5.5
1	H	199	SER	5.5
1	G	487	LEU	5.5
1	H	405	ALA	5.5
1	E	137	LYS	5.4
1	B	258	ASN	5.4
1	B	260	ASN	5.4
1	B	558	ALA	5.4
1	K	153	VAL	5.4
1	L	132	VAL	5.4
1	G	222	LEU	5.4
1	L	583	PHE	5.4
1	E	548	SER	5.4
1	B	112	VAL	5.4
1	B	318	ALA	5.4
1	G	112	VAL	5.4
1	F	152	GLN	5.4
1	J	94	LEU	5.4
1	E	446	THR	5.4
1	B	175	PHE	5.4
1	K	100	PRO	5.4
1	H	233	ASN	5.4
1	K	420	ASN	5.4
1	E	510	ILE	5.4
1	L	117	ILE	5.4
1	B	330	VAL	5.4
1	H	167	VAL	5.4
1	H	390	GLY	5.4
1	J	595	LEU	5.4
1	B	410	ALA	5.4
1	B	308	VAL	5.4
1	F	195	VAL	5.4
1	F	286	VAL	5.4
1	F	323	LEU	5.4
1	F	581	TRP	5.4
1	G	214	LEU	5.4
1	G	385	LEU	5.4

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Mol	Chain	Res	Type	RSRZ
1	I	595	LEU	5.4
1	H	277	TYR	5.4
1	J	335	GLU	5.4
1	K	282	GLU	5.4
1	I	204	LYS	5.4
1	F	186	ALA	5.4
1	A	537	LEU	5.4
1	E	330	VAL	5.4
1	G	603	ASP	5.4
1	J	114	VAL	5.4
1	C	555	SER	5.4
1	H	163	GLU	5.4
1	I	261	MET	5.4
1	H	110	ILE	5.3
1	I	264	ILE	5.3
1	A	104[A]	ASN	5.3
1	C	385	LEU	5.3
1	G	391	SER	5.3
1	J	297	LEU	5.3
1	J	426	LEU	5.3
1	L	219	LEU	5.3
1	F	362	LYS	5.3
1	L	398	PHE	5.3
1	I	363	GLY	5.3
1	G	577	ALA	5.3
1	H	602	ASN	5.3
1	I	377	THR	5.3
1	H	153	VAL	5.3
1	I	308	VAL	5.3
1	I	310	LEU	5.3
1	A	257	LYS	5.3
1	H	203	MET	5.3
1	I	134	ASN	5.3
1	I	274	ALA	5.3
1	B	205	ARG	5.3
1	A	219	LEU	5.3
1	L	470	LEU	5.3
1	F	187	VAL	5.3
1	G	136	GLY	5.3
1	L	329	GLY	5.3
1	F	571	TRP	5.3
1	G	526	TRP	5.3

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Mol	Chain	Res	Type	RSRZ
1	A	298	ILE	5.3
1	G	393	ILE	5.3
1	J	262	GLU	5.3
1	D	395	LEU	5.3
1	F	297	LEU	5.3
1	A	551	VAL	5.3
1	E	281	VAL	5.3
1	C	462	GLY	5.3
1	G	392	MET	5.3
1	H	313	ALA	5.3
1	I	271	ILE	5.3
1	C	601	LEU	5.3
1	H	140	GLY	5.3
1	K	495	LEU	5.3
1	D	511	ASN	5.3
1	H	259	VAL	5.3
1	I	566	VAL	5.3
1	C	565	PHE	5.3
1	H	485	ALA	5.3
1	H	197	ASP	5.3
1	F	263	TYR	5.3
1	H	472	TYR	5.3
1	D	149	ASN	5.3
1	A	426	LEU	5.3
1	I	259	VAL	5.2
1	H	302	SER	5.2
1	A	581	TRP	5.2
1	K	191	GLY	5.2
1	F	493	TYR	5.2
1	A	549	SER	5.2
1	K	490	ALA	5.2
1	E	106	PRO	5.2
1	G	354	PHE	5.2
1	G	119	GLY	5.2
1	I	477	GLY	5.2
1	E	99	ILE	5.2
1	E	117	ILE	5.2
1	H	228	ILE	5.2
1	L	157	LEU	5.2
1	D	148	VAL	5.2
1	F	435	SER	5.2
1	H	478	VAL	5.2

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Mol	Chain	Res	Type	RSRZ
1	B	193	GLY	5.2
1	C	400	MET	5.2
1	D	412	CYS	5.2
1	F	223	THR	5.2
1	C	393	ILE	5.2
1	E	445	ILE	5.2
1	H	484	ILE	5.2
1	K	484	ILE	5.2
1	H	364	ASP	5.2
1	E	277	TYR	5.2
1	G	480	TYR	5.2
1	L	480	TYR	5.2
1	E	362	LYS	5.2
1	K	148	VAL	5.2
1	G	135	PRO	5.2
1	E	275	ASP	5.2
1	A	107	ILE	5.2
1	G	144	ILE	5.2
1	H	362	LYS	5.2
1	I	107	ILE	5.2
1	L	298	ILE	5.2
1	G	146	SER	5.2
1	K	297	LEU	5.2
1	B	439	TYR	5.2
1	L	277	TYR	5.2
1	A	206	VAL	5.2
1	B	482	VAL	5.2
1	I	478	VAL	5.2
1	G	462	GLY	5.2
1	A	274	ALA	5.2
1	K	405	ALA	5.2
1	L	577	ALA	5.2
1	A	109	ASP	5.2
1	F	491	MET	5.2
1	J	164	LYS	5.2
1	C	423	ILE	5.2
1	F	101	ILE	5.2
1	A	511	ASN	5.2
1	J	280	GLU	5.2
1	A	365	VAL	5.2
1	K	486	THR	5.1
1	G	582	ASN	5.1

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Mol	Chain	Res	Type	RSRZ
1	I	133	ASN	5.1
1	A	546	GLN	5.1
1	A	407	LEU	5.1
1	D	297	LEU	5.1
1	F	198	LEU	5.1
1	G	239	LEU	5.1
1	D	261	MET	5.1
1	G	107	ILE	5.1
1	C	275	ASP	5.1
1	J	239	LEU	5.1
1	L	231	ASP	5.1
1	D	187	VAL	5.1
1	J	230	VAL	5.1
1	L	195	VAL	5.1
1	L	340	ALA	5.1
1	A	452	THR	5.1
1	F	273	ASN	5.1
1	D	363	GLY	5.1
1	E	237	PHE	5.1
1	C	376	ILE	5.1
1	G	544	ILE	5.1
1	G	547	ILE	5.1
1	K	363	GLY	5.1
1	C	183	ASN	5.1
1	F	304	TYR	5.1
1	F	405	ALA	5.1
1	G	315	VAL	5.1
1	I	287	TYR	5.1
1	I	411	TYR	5.1
1	E	550	SER	5.1
1	L	199	SER	5.1
1	I	364	ASP	5.1
1	I	333	LEU	5.1
1	J	495	LEU	5.1
1	A	167	VAL	5.1
1	E	429	VAL	5.1
1	A	391	SER	5.1
1	E	541	TYR	5.1
1	G	372	VAL	5.1
1	J	488	THR	5.1
1	H	205	ARG	5.1
1	C	192	CYS	5.1

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Mol	Chain	Res	Type	RSRZ
1	B	183	ASN	5.1
1	B	371	LEU	5.1
1	C	273	ASN	5.1
1	F	219	LEU	5.1
1	F	562	LEU	5.1
1	H	492	LEU	5.1
1	I	242	LEU	5.1
1	H	274	ALA	5.1
1	C	207	VAL	5.1
1	K	315	VAL	5.1
1	C	290	GLY	5.1
1	J	411	TYR	5.1
1	L	189	TYR	5.1
1	C	162	MET	5.1
1	H	571	TRP	5.1
1	I	183	ASN	5.1
1	C	323	LEU	5.0
1	F	470	LEU	5.0
1	L	379	ASP	5.0
1	G	145	SER	5.0
1	L	486	THR	5.0
1	B	259	VAL	5.0
1	G	362	LYS	5.0
1	A	530	ILE	5.0
1	C	305	CYS	5.0
1	D	369	ILE	5.0
1	K	101	ILE	5.0
1	I	514	LEU	5.0
1	F	488	THR	5.0
1	G	402	GLY	5.0
1	J	299	ALA	5.0
1	K	340	ALA	5.0
1	F	281	VAL	5.0
1	L	289	PHE	5.0
1	A	154	SER	5.0
1	L	94	LEU	5.0
1	G	275	ASP	5.0
1	K	434	VAL	5.0
1	K	557	VAL	5.0
1	I	247	MET	5.0
1	J	349	MET	5.0
1	A	515	GLN	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	144	ILE	5.0
1	B	599	PHE	5.0
1	K	311	SER	5.0
1	K	549	SER	5.0
1	G	137	LYS	5.0
1	I	198	LEU	5.0
1	B	467	ALA	5.0
1	G	128	THR	5.0
1	K	274	ALA	5.0
1	E	406	VAL	5.0
1	G	579	VAL	5.0
1	J	557	VAL	5.0
1	K	207	VAL	5.0
1	A	400	MET	5.0
1	E	349	MET	5.0
1	J	261	MET	5.0
1	C	292	TYR	5.0
1	G	499	TYR	5.0
1	D	549	SER	5.0
1	I	580	SER	5.0
1	F	576	ILE	5.0
1	B	333	LEU	5.0
1	C	404	ALA	5.0
1	F	452	THR	5.0
1	H	322	ASN	5.0
1	J	430	CYS	5.0
1	A	372	VAL	5.0
1	D	551	VAL	5.0
1	K	524	VAL	5.0
1	C	247	MET	5.0
1	F	146	SER	5.0
1	A	246	TYR	5.0
1	G	263	TYR	5.0
1	A	271	ILE	5.0
1	H	226	PHE	5.0
1	H	445	ILE	5.0
1	B	597	THR	5.0
1	H	385	LEU	5.0
1	I	276	THR	5.0
1	L	237	PHE	5.0
1	C	135	PRO	4.9
1	A	87	GLU	4.9

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Mol	Chain	Res	Type	RSRZ
1	L	162	MET	4.9
1	B	117	ILE	4.9
1	F	113	GLN	4.9
1	C	165	PHE	4.9
1	J	376	ILE	4.9
1	J	467	ALA	4.9
1	L	465	THR	4.9
1	G	297	LEU	4.9
1	G	596	LEU	4.9
1	K	487	LEU	4.9
1	G	389	PRO	4.9
1	G	434	VAL	4.9
1	H	181	ASN	4.9
1	H	336	LEU	4.9
1	J	219	LEU	4.9
1	L	321	LEU	4.9
1	C	256	ASP	4.9
1	E	140	GLY	4.9
1	D	185	VAL	4.9
1	D	211	VAL	4.9
1	C	486	THR	4.9
1	A	313	ALA	4.9
1	D	439	TYR	4.9
1	F	277	TYR	4.9
1	I	553	ALA	4.9
1	A	393	ILE	4.9
1	H	393	ILE	4.9
1	I	376	ILE	4.9
1	G	583	PHE	4.9
1	L	395	LEU	4.9
1	L	426	LEU	4.9
1	F	154	SER	4.9
1	J	389	PRO	4.9
1	K	166	ASN	4.9
1	L	126	GLY	4.9
1	F	507	GLU	4.9
1	G	123	VAL	4.9
1	K	308	VAL	4.9
1	G	266	HIS	4.9
1	I	171	THR	4.9
1	K	291	THR	4.9
1	L	473	ALA	4.9

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Mol	Chain	Res	Type	RSRZ
1	C	537	LEU	4.9
1	D	192	CYS	4.9
1	D	409	CYS	4.9
1	D	472	TYR	4.9
1	D	273	ASN	4.9
1	F	328	LEU	4.9
1	K	492	LEU	4.9
1	F	289	PHE	4.9
1	A	112	VAL	4.9
1	C	344	VAL	4.9
1	D	429	VAL	4.9
1	F	421	VAL	4.9
1	H	190	VAL	4.9
1	K	593	VAL	4.9
1	C	248	THR	4.9
1	B	393	ILE	4.9
1	F	466	LEU	4.9
1	J	574	ILE	4.9
1	C	121	CYS	4.9
1	I	238	PHE	4.9
1	L	561	PHE	4.9
1	C	200	GLU	4.9
1	C	229	ASN	4.9
1	E	569	THR	4.9
1	A	460	ALA	4.8
1	G	473	ALA	4.8
1	A	198	LEU	4.8
1	A	264	ILE	4.8
1	A	376	ILE	4.8
1	B	107	ILE	4.8
1	C	228	ILE	4.8
1	F	129	ILE	4.8
1	C	493	TYR	4.8
1	G	244	TYR	4.8
1	K	541	TYR	4.8
1	K	155	GLU	4.8
1	A	197	ASP	4.8
1	B	365	VAL	4.8
1	G	258	ASN	4.8
1	H	551	VAL	4.8
1	I	92	VAL	4.8
1	A	486	THR	4.8

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Mol	Chain	Res	Type	RSRZ
1	B	105	THR	4.8
1	E	291	THR	4.8
1	E	382	GLY	4.8
1	K	485	ALA	4.8
1	J	550	SER	4.8
1	J	135	PRO	4.8
1	E	507	GLU	4.8
1	I	262	GLU	4.8
1	F	287	TYR	4.8
1	F	583	PHE	4.8
1	I	130	PHE	4.8
1	K	398	PHE	4.8
1	A	195	VAL	4.8
1	C	550	SER	4.8
1	E	558	ALA	4.8
1	K	559	SER	4.8
1	C	150	ASP	4.8
1	E	210	LEU	4.8
1	F	99	ILE	4.8
1	G	514	LEU	4.8
1	H	357	LEU	4.8
1	K	117	ILE	4.8
1	I	591	PHE	4.8
1	I	88	VAL	4.8
1	J	403	CYS	4.8
1	J	549	SER	4.8
1	B	180	ASP	4.8
1	C	298	ILE	4.8
1	D	487	LEU	4.8
1	F	115	TYR	4.8
1	E	504	GLY	4.8
1	G	268	GLY	4.8
1	L	140	GLY	4.8
1	G	276	THR	4.8
1	A	286	VAL	4.8
1	B	396	MET	4.8
1	D	524	VAL	4.8
1	D	557	VAL	4.8
1	E	577	ALA	4.8
1	H	206	VAL	4.8
1	H	428	ALA	4.8
1	I	490	ALA	4.8

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Mol	Chain	Res	Type	RSRZ
1	C	181	ASN	4.8
1	H	174	HIS	4.8
1	J	229	ASN	4.8
1	E	487	LEU	4.8
1	E	492	LEU	4.8
1	A	547	ILE	4.8
1	D	544	ILE	4.8
1	G	115	TYR	4.8
1	H	116	ASP	4.8
1	C	276	THR	4.8
1	D	486	THR	4.8
1	B	207	VAL	4.8
1	I	211	VAL	4.8
1	G	169	LEU	4.8
1	G	331	LYS	4.8
1	H	219	LEU	4.8
1	I	357	LEU	4.8
1	G	186	ALA	4.7
1	H	258	ASN	4.7
1	L	387	ALA	4.7
1	L	478	VAL	4.7
1	C	381	GLY	4.7
1	I	197	ASP	4.7
1	K	547	ILE	4.7
1	A	561	PHE	4.7
1	F	156	PHE	4.7
1	C	141	PRO	4.7
1	E	383	TYR	4.7
1	G	588	PRO	4.7
1	C	286	VAL	4.7
1	B	323	LEU	4.7
1	L	528	PRO	4.7
1	D	138	GLU	4.7
1	I	473	ALA	4.7
1	I	392	MET	4.7
1	E	309	SER	4.7
1	H	371	LEU	4.7
1	H	179	ASN	4.7
1	L	107	ILE	4.7
1	E	121	CYS	4.7
1	L	409	CYS	4.7
1	D	387	ALA	4.7

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Mol	Chain	Res	Type	RSRZ
1	G	543	ASP	4.7
1	I	299	ALA	4.7
1	D	390	GLY	4.7
1	E	292	TYR	4.7
1	E	373	GLY	4.7
1	J	493	TYR	4.7
1	K	578	GLY	4.7
1	E	524	VAL	4.7
1	F	551	VAL	4.7
1	I	344	VAL	4.7
1	J	88	VAL	4.7
1	K	195	VAL	4.7
1	H	127	LEU	4.7
1	B	110	ILE	4.7
1	B	513	ILE	4.7
1	G	129	ILE	4.7
1	L	529	ILE	4.7
1	E	276	THR	4.7
1	I	150	ASP	4.7
1	L	418	PRO	4.7
1	B	331	LYS	4.7
1	B	362	LYS	4.7
1	F	118	LYS	4.7
1	J	599	PHE	4.7
1	K	175	PHE	4.7
1	L	552	LYS	4.7
1	K	192	CYS	4.7
1	B	472	TYR	4.7
1	H	293	TYR	4.7
1	J	400	MET	4.7
1	B	566	VAL	4.7
1	G	229	ASN	4.7
1	H	195	VAL	4.7
1	I	365	VAL	4.7
1	J	455	VAL	4.7
1	K	401	SER	4.7
1	L	123	VAL	4.7
1	B	137	LYS	4.7
1	B	174	HIS	4.7
1	E	355	ILE	4.7
1	L	556	ILE	4.7
1	I	100	PRO	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	280	GLU	4.7
1	E	398	PHE	4.7
1	F	558	ALA	4.7
1	H	403	CYS	4.6
1	J	305	CYS	4.6
1	K	409	CYS	4.6
1	E	520	SER	4.6
1	K	550	SER	4.6
1	K	482	VAL	4.6
1	L	286	VAL	4.6
1	H	271	ILE	4.6
1	J	513	ILE	4.6
1	K	393	ILE	4.6
1	C	583	PHE	4.6
1	A	584	LYS	4.6
1	B	203	MET	4.6
1	D	197	ASP	4.6
1	A	403	CYS	4.6
1	G	413	VAL	4.6
1	K	190	VAL	4.6
1	D	495	LEU	4.6
1	E	495	LEU	4.6
1	H	297	LEU	4.6
1	L	466	LEU	4.6
1	A	496	GLY	4.6
1	C	296	GLN	4.6
1	D	376	ILE	4.6
1	E	453	ILE	4.6
1	H	556	ILE	4.6
1	L	276	THR	4.6
1	L	444	ILE	4.6
1	F	582	ASN	4.6
1	H	511	ASN	4.6
1	D	178	PHE	4.6
1	H	387	ALA	4.6
1	J	410	ALA	4.6
1	L	565	PHE	4.6
1	D	279	GLU	4.6
1	E	559	SER	4.6
1	F	394	ASP	4.6
1	A	330	VAL	4.6
1	E	385	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
1	F	395	LEU	4.6
1	F	596	LEU	4.6
1	G	127	LEU	4.6
1	H	351	PRO	4.6
1	L	169	LEU	4.6
1	L	537	LEU	4.6
1	D	228	ILE	4.6
1	L	149	ASN	4.6
1	B	340	ALA	4.6
1	B	364	ASP	4.6
1	L	460	ALA	4.6
1	A	392	MET	4.6
1	C	257	LYS	4.6
1	D	203	MET	4.6
1	E	278	LYS	4.6
1	G	589	LYS	4.6
1	I	396	MET	4.6
1	E	592	GLY	4.6
1	E	593	VAL	4.6
1	J	551	VAL	4.6
1	L	533	TYR	4.6
1	A	134	ASN	4.6
1	A	385	LEU	4.6
1	B	395	LEU	4.6
1	G	291	THR	4.6
1	G	395	LEU	4.6
1	L	242	LEU	4.6
1	L	333	LEU	4.6
1	L	488	THR	4.6
1	F	298	ILE	4.6
1	C	405	ALA	4.6
1	D	401	SER	4.6
1	I	196	ALA	4.6
1	K	220	SER	4.6
1	L	451	LYS	4.6
1	K	392	MET	4.6
1	C	322	ASN	4.6
1	F	136	GLY	4.6
1	F	402	GLY	4.6
1	J	272	ASN	4.6
1	K	390	GLY	4.6
1	B	114	VAL	4.6

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Mol	Chain	Res	Type	RSRZ
1	E	365	VAL	4.6
1	G	301	PRO	4.6
1	G	593	VAL	4.6
1	J	478	VAL	4.6
1	L	455	VAL	4.6
1	E	493	TYR	4.6
1	F	242	LEU	4.6
1	L	342	LEU	4.6
1	D	294	ALA	4.6
1	E	196	ALA	4.6
1	H	227	GLU	4.6
1	C	252	PHE	4.6
1	D	378	PHE	4.6
1	E	425	PHE	4.6
1	E	581	TRP	4.6
1	D	233	ASN	4.6
1	F	432	ASN	4.6
1	A	434	VAL	4.6
1	C	502	VAL	4.6
1	D	207	VAL	4.6
1	F	315	VAL	4.6
1	I	524	VAL	4.6
1	K	248	THR	4.6
1	L	182	LYS	4.6
1	L	551	VAL	4.6
1	A	342	LEU	4.6
1	A	439	TYR	4.6
1	B	267	LEU	4.6
1	C	514	LEU	4.6
1	E	537	LEU	4.6
1	G	323	LEU	4.6
1	J	466	LEU	4.6
1	A	453	ILE	4.5
1	J	542	ALA	4.5
1	F	409	CYS	4.5
1	B	116	ASP	4.5
1	J	450	GLY	4.5
1	B	433	MET	4.5
1	B	372	VAL	4.5
1	C	434	VAL	4.5
1	L	330	VAL	4.5
1	L	600	VAL	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	263	TYR	4.5
1	D	470	LEU	4.5
1	A	473	ALA	4.5
1	H	473	ALA	4.5
1	H	585	ALA	4.5
1	J	99	ILE	4.5
1	L	274	ALA	4.5
1	L	453	ILE	4.5
1	B	602	ASN	4.5
1	E	345	GLY	4.5
1	I	275	ASP	4.5
1	I	252	PHE	4.5
1	G	396	MET	4.5
1	B	539	SER	4.5
1	G	248	THR	4.5
1	I	434	VAL	4.5
1	J	579	VAL	4.5
1	L	146	SER	4.5
1	G	357	LEU	4.5
1	A	287	TYR	4.5
1	A	329	GLY	4.5
1	A	445	ILE	4.5
1	G	381	GLY	4.5
1	G	565	PHE	4.5
1	A	111	LYS	4.5
1	J	192	CYS	4.5
1	D	180	ASP	4.5
1	E	230	VAL	4.5
1	G	256	ASP	4.5
1	G	407	LEU	4.5
1	H	242	LEU	4.5
1	H	429	VAL	4.5
1	K	407	LEU	4.5
1	B	300	ALA	4.5
1	B	370	ALA	4.5
1	B	477	GLY	4.5
1	E	300	ALA	4.5
1	H	176	TYR	4.5
1	H	477	GLY	4.5
1	I	300	ALA	4.5
1	K	188	GLY	4.5
1	H	398	PHE	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	223	THR	4.5
1	F	177	MET	4.5
1	B	159	ASP	4.5
1	G	171	THR	4.5
1	B	179	ASN	4.5
1	A	211	VAL	4.5
1	C	450	GLY	4.5
1	G	219	LEU	4.5
1	G	310	LEU	4.5
1	G	464	LEU	4.5
1	I	317	LEU	4.5
1	K	579	VAL	4.5
1	H	425	PHE	4.5
1	K	583	PHE	4.5
1	C	338	MET	4.5
1	E	486	THR	4.5
1	H	161	ASN	4.5
1	K	396	MET	4.5
1	C	466	LEU	4.5
1	I	372	VAL	4.5
1	K	224	VAL	4.5
1	L	365	VAL	4.5
1	L	579	VAL	4.5
1	D	467	ALA	4.5
1	J	405	ALA	4.5
1	L	313	ALA	4.5
1	E	528	PRO	4.5
1	C	394	ASP	4.5
1	L	116	ASP	4.5
1	C	494	SER	4.4
1	D	86	SER	4.4
1	J	517	SER	4.4
1	K	348	SER	4.4
1	F	486	THR	4.4
1	J	552	LYS	4.4
1	L	158	LYS	4.4
1	A	224	VAL	4.4
1	B	514	LEU	4.4
1	C	153	VAL	4.4
1	F	190	VAL	4.4
1	F	404	ALA	4.4
1	G	387	ALA	4.4

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Mol	Chain	Res	Type	RSRZ
1	I	537	LEU	4.4
1	K	313	ALA	4.4
1	L	214	LEU	4.4
1	C	543	ASP	4.4
1	D	484	ILE	4.4
1	B	176	TYR	4.4
1	F	472	TYR	4.4
1	K	115	TYR	4.4
1	L	341	TYR	4.4
1	F	276	THR	4.4
1	G	382	GLY	4.4
1	G	561	PHE	4.4
1	A	470	LEU	4.4
1	C	387	ALA	4.4
1	C	542	ALA	4.4
1	C	557	VAL	4.4
1	H	169	LEU	4.4
1	J	85	ALA	4.4
1	L	207	VAL	4.4
1	A	137	LYS	4.4
1	I	589	LYS	4.4
1	E	295	SER	4.4
1	A	430	CYS	4.4
1	C	541	TYR	4.4
1	B	171	THR	4.4
1	G	592	GLY	4.4
1	B	398	PHE	4.4
1	L	130	PHE	4.4
1	B	366	LYS	4.4
1	C	364	ASP	4.4
1	I	379	ASP	4.4
1	A	314	ALA	4.4
1	A	467	ALA	4.4
1	C	577	ALA	4.4
1	E	306	ASN	4.4
1	H	131	LEU	4.4
1	H	214	LEU	4.4
1	I	148	VAL	4.4
1	I	330	VAL	4.4
1	L	139	ASN	4.4
1	C	510	ILE	4.4
1	K	298	ILE	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	462	GLY	4.4
1	F	347	GLY	4.4
1	A	412	CYS	4.4
1	G	552	LYS	4.4
1	G	138	GLU	4.4
1	H	152	GLN	4.4
1	G	285	ARG	4.4
1	K	306	ASN	4.4
1	C	294	ALA	4.4
1	F	585	ALA	4.4
1	A	239	LEU	4.4
1	C	495	LEU	4.4
1	F	321	LEU	4.4
1	L	187	VAL	4.4
1	L	224	VAL	4.4
1	D	147	LYS	4.4
1	F	119	GLY	4.4
1	G	111	LYS	4.4
1	J	529	ILE	4.4
1	B	248	THR	4.4
1	C	171	THR	4.4
1	K	488	THR	4.4
1	I	115	TYR	4.4
1	L	383	TYR	4.4
1	K	581	TRP	4.4
1	A	531	ASN	4.4
1	B	457	ASN	4.4
1	D	599	PHE	4.4
1	H	162	MET	4.4
1	H	247	MET	4.4
1	K	432	ASN	4.4
1	C	410	ALA	4.4
1	D	318	ALA	4.4
1	E	343	SER	4.4
1	C	151	LYS	4.4
1	E	562	LEU	4.4
1	K	184	SER	4.4
1	K	362	LYS	4.4
1	A	308	VAL	4.4
1	H	524	VAL	4.4
1	J	185	VAL	4.4
1	H	462	GLY	4.4

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Mol	Chain	Res	Type	RSRZ
1	L	268	GLY	4.4
1	A	180	ASP	4.4
1	A	574	ILE	4.4
1	G	484	ILE	4.4
1	H	538	ASN	4.4
1	D	244	TYR	4.4
1	F	499	TYR	4.4
1	A	203	MET	4.4
1	E	354	PHE	4.4
1	A	469	ALA	4.4
1	A	553	ALA	4.4
1	G	295	SER	4.4
1	G	447	ALA	4.4
1	I	201	ALA	4.4
1	K	441	PRO	4.4
1	L	192	CYS	4.4
1	L	558	ALA	4.4
1	A	127	LEU	4.3
1	A	456	GLY	4.3
1	E	464	LEU	4.3
1	H	328	LEU	4.3
1	I	406	VAL	4.3
1	L	225	VAL	4.3
1	A	423	ILE	4.3
1	B	298	ILE	4.3
1	A	361	SER	4.3
1	H	301	PRO	4.3
1	F	485	ALA	4.3
1	I	526	TRP	4.3
1	H	440	ARG	4.3
1	K	275	ASP	4.3
1	K	339	GLY	4.3
1	A	464	LEU	4.3
1	I	562	LEU	4.3
1	J	596	LEU	4.3
1	F	593	VAL	4.3
1	L	344	VAL	4.3
1	L	372	VAL	4.3
1	G	118	LYS	4.3
1	F	529	ILE	4.3
1	G	110	ILE	4.3
1	G	376	ILE	4.3

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Mol	Chain	Res	Type	RSRZ
1	L	445	ILE	4.3
1	A	145	SER	4.3
1	B	95	ASP	4.3
1	E	401	SER	4.3
1	K	113	GLN	4.3
1	H	433	MET	4.3
1	B	504	GLY	4.3
1	F	373	GLY	4.3
1	F	553	ALA	4.3
1	C	417	LYS	4.3
1	A	210	LEU	4.3
1	A	560	LEU	4.3
1	B	297	LEU	4.3
1	B	464	LEU	4.3
1	H	466	LEU	4.3
1	A	225	VAL	4.3
1	B	230	VAL	4.3
1	G	167	VAL	4.3
1	G	264	ILE	4.3
1	B	140	GLY	4.3
1	I	329	GLY	4.3
1	K	408	GLY	4.3
1	A	383	TYR	4.3
1	E	404	ALA	4.3
1	G	201	ALA	4.3
1	G	469	ALA	4.3
1	I	103	TYR	4.3
1	B	217	ASN	4.3
1	I	601	LEU	4.3
1	D	337	LYS	4.3
1	J	150	ASP	4.3
1	E	298	ILE	4.3
1	E	544	ILE	4.3
1	B	418	PRO	4.3
1	F	462	GLY	4.3
1	H	191	GLY	4.3
1	H	410	ALA	4.3
1	L	294	ALA	4.3
1	A	115	TYR	4.3
1	A	156	PHE	4.3
1	A	176	TYR	4.3
1	A	480	TYR	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	599	PHE	4.3
1	D	541	TYR	4.3
1	H	439	TYR	4.3
1	L	270	TYR	4.3
1	E	560	LEU	4.3
1	H	395	LEU	4.3
1	L	371	LEU	4.3
1	D	552	LYS	4.3
1	D	419	GLU	4.3
1	G	142	VAL	4.3
1	B	101	ILE	4.3
1	C	99	ILE	4.3
1	D	391	SER	4.3
1	D	448	SER	4.3
1	G	298	ILE	4.3
1	J	361	SER	4.3
1	J	412	CYS	4.3
1	A	139	ASN	4.3
1	E	521	ASN	4.3
1	H	133	ASN	4.3
1	C	261	MET	4.3
1	F	314	ALA	4.3
1	L	490	ALA	4.3
1	B	378	PHE	4.3
1	D	493	TYR	4.3
1	E	472	TYR	4.3
1	I	165	PHE	4.3
1	I	288	TYR	4.3
1	B	222	LEU	4.3
1	B	479	ASP	4.3
1	C	197	ASP	4.3
1	D	210	LEU	4.3
1	G	180	ASP	4.3
1	B	302	SER	4.3
1	D	88	VAL	4.3
1	F	557	VAL	4.3
1	G	254	SER	4.3
1	A	322	ASN	4.2
1	D	449	ASN	4.2
1	E	272	ASN	4.2
1	H	444	ILE	4.2
1	I	547	ILE	4.2

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Mol	Chain	Res	Type	RSRZ
1	I	582	ASN	4.2
1	D	137	LYS	4.2
1	H	337	LYS	4.2
1	L	394	ASP	4.2
1	A	466	LEU	4.2
1	B	411	TYR	4.2
1	I	94	LEU	4.2
1	C	97	THR	4.2
1	K	361	SER	4.2
1	K	504	GLY	4.2
1	A	272	ASN	4.2
1	E	312	ASN	4.2
1	F	372	VAL	4.2
1	H	111	LYS	4.2
1	H	112	VAL	4.2
1	A	389	PRO	4.2
1	E	393	ILE	4.2
1	H	510	ILE	4.2
1	J	556	ILE	4.2
1	A	535	ALA	4.2
1	C	313	ALA	4.2
1	G	412	CYS	4.2
1	H	305	CYS	4.2
1	J	392	MET	4.2
1	F	237	PHE	4.2
1	A	133	ASN	4.2
1	A	229	ASN	4.2
1	E	361	SER	4.2
1	I	347	GLY	4.2
1	I	465	THR	4.2
1	L	472	TYR	4.2
1	C	185	VAL	4.2
1	I	593	VAL	4.2
1	K	206	VAL	4.2
1	H	479	ASP	4.2
1	B	405	ALA	4.2
1	D	490	ALA	4.2
1	E	318	ALA	4.2
1	C	143	LYS	4.2
1	I	163	GLU	4.2
1	A	591	PHE	4.2
1	B	517	SER	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	565	PHE	4.2
1	F	161	ASN	4.2
1	F	412	CYS	4.2
1	G	580	SER	4.2
1	H	599	PHE	4.2
1	J	260	ASN	4.2
1	D	385	LEU	4.2
1	D	492	LEU	4.2
1	E	595	LEU	4.2
1	K	302	SER	4.2
1	B	108	HIS	4.2
1	C	308	VAL	4.2
1	K	455	VAL	4.2
1	J	101	ILE	4.2
1	L	355	ILE	4.2
1	L	484	ILE	4.2
1	A	382	GLY	4.2
1	A	396	MET	4.2
1	B	273	ASN	4.2
1	J	104	ASN	4.2
1	J	348	SER	4.2
1	L	592	GLY	4.2
1	A	248	THR	4.2
1	A	378	PHE	4.2
1	C	94	LEU	4.2
1	D	243	PHE	4.2
1	E	470	LEU	4.2
1	F	169	LEU	4.2
1	H	171	THR	4.2
1	H	310	LEU	4.2
1	I	371	LEU	4.2
1	K	202	ASP	4.2
1	K	426	LEU	4.2
1	K	503	PHE	4.2
1	K	596	LEU	4.2
1	G	121	CYS	4.2
1	B	232	LYS	4.2
1	C	411	TYR	4.2
1	E	115	TYR	4.2
1	F	533	TYR	4.2
1	G	176	TYR	4.2
1	I	472	TYR	4.2

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Mol	Chain	Res	Type	RSRZ
1	K	307	PRO	4.2
1	J	331	LYS	4.2
1	B	88	VAL	4.2
1	E	153	VAL	4.2
1	G	558	ALA	4.2
1	K	299	ALA	4.2
1	L	515	GLN	4.2
1	L	576	ILE	4.2
1	D	457	ASN	4.2
1	G	260	ASN	4.2
1	E	119	GLY	4.2
1	C	295	SER	4.2
1	C	311	SER	4.2
1	G	162	MET	4.2
1	H	172	SER	4.2
1	H	184	SER	4.2
1	K	295	SER	4.2
1	L	526	TRP	4.2
1	L	459	ASP	4.2
1	G	257	LYS	4.2
1	G	488	THR	4.2
1	K	417	LYS	4.2
1	K	597	THR	4.2
1	G	175	PHE	4.2
1	H	565	PHE	4.2
1	I	426	LEU	4.2
1	K	96	PRO	4.2
1	L	127	LEU	4.2
1	L	495	LEU	4.2
1	H	263	TYR	4.2
1	H	383	TYR	4.2
1	C	471	VAL	4.2
1	E	478	VAL	4.2
1	F	429	VAL	4.2
1	I	502	VAL	4.2
1	C	258	ASN	4.2
1	G	273	ASN	4.2
1	A	299	ALA	4.2
1	A	387	ALA	4.2
1	A	500	ALA	4.2
1	E	556	ILE	4.2
1	J	186	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	158	LYS	4.2
1	C	146	SER	4.2
1	C	232	LYS	4.2
1	D	302	SER	4.2
1	E	311	SER	4.2
1	I	180	ASP	4.2
1	A	569	THR	4.1
1	D	377	THR	4.1
1	C	307	PRO	4.1
1	E	94	LEU	4.1
1	I	234	LEU	4.1
1	F	176	TYR	4.1
1	K	122	ASN	4.1
1	A	471	VAL	4.1
1	H	421	VAL	4.1
1	I	281	VAL	4.1
1	I	421	VAL	4.1
1	J	138	GLU	4.1
1	J	195	VAL	4.1
1	A	592	GLY	4.1
1	J	390	GLY	4.1
1	E	513	ILE	4.1
1	I	484	ILE	4.1
1	L	491	MET	4.1
1	A	297	LEU	4.1
1	A	571	TRP	4.1
1	C	210	LEU	4.1
1	C	464	LEU	4.1
1	E	357	LEU	4.1
1	F	426	LEU	4.1
1	G	470	LEU	4.1
1	I	398	PHE	4.1
1	I	487	LEU	4.1
1	I	495	LEU	4.1
1	B	164	LYS	4.1
1	B	511	ASN	4.1
1	C	457	ASN	4.1
1	D	229	ASN	4.1
1	G	134	ASN	4.1
1	J	384	ASN	4.1
1	K	602	ASN	4.1
1	C	148	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	533	TYR	4.1
1	K	502	VAL	4.1
1	L	566	VAL	4.1
1	A	405	ALA	4.1
1	C	428	ALA	4.1
1	E	369	ILE	4.1
1	A	162	MET	4.1
1	E	419	GLU	4.1
1	G	158	LYS	4.1
1	K	106	PRO	4.1
1	D	601	LEU	4.1
1	F	127	LEU	4.1
1	H	139	ASN	4.1
1	H	560	LEU	4.1
1	E	565	PHE	4.1
1	G	120	GLY	4.1
1	B	142	VAL	4.1
1	E	172	SER	4.1
1	H	281	VAL	4.1
1	I	145	SER	4.1
1	F	542	ALA	4.1
1	I	195	VAL	4.1
1	L	287	TYR	4.1
1	L	406	VAL	4.1
1	B	369	ILE	4.1
1	B	417	LYS	4.1
1	C	107	ILE	4.1
1	G	574	ILE	4.1
1	L	508	GLU	4.1
1	B	412	CYS	4.1
1	A	602	ASN	4.1
1	D	488	THR	4.1
1	E	505	ASN	4.1
1	J	105	THR	4.1
1	A	379	ASP	4.1
1	G	159	ASP	4.1
1	A	234	LEU	4.1
1	A	357	LEU	4.1
1	C	591	PHE	4.1
1	E	290	GLY	4.1
1	I	408	GLY	4.1
1	A	494	SER	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	194	SER	4.1
1	G	581	TRP	4.1
1	I	581	TRP	4.1
1	L	571	TRP	4.1
1	B	404	ALA	4.1
1	B	189	TYR	4.1
1	E	92	VAL	4.1
1	F	344	VAL	4.1
1	J	112	VAL	4.1
1	L	359	TYR	4.1
1	L	574	ILE	4.1
1	I	441	PRO	4.1
1	H	465	THR	4.1
1	F	162	MET	4.1
1	I	213	MET	4.1
1	B	595	LEU	4.1
1	H	596	LEU	4.1
1	I	560	LEU	4.1
1	J	509	LEU	4.1
1	K	119	GLY	4.1
1	D	209	SER	4.1
1	G	378	PHE	4.1
1	L	391	SER	4.1
1	C	330	VAL	4.1
1	F	134	ASN	4.1
1	G	350	TYR	4.1
1	I	244	TYR	4.1
1	I	499	TYR	4.1
1	A	377	THR	4.1
1	G	255	THR	4.1
1	K	518	LYS	4.1
1	A	433	MET	4.1
1	C	119	GLY	4.1
1	C	140	GLY	4.1
1	D	592	GLY	4.1
1	C	333	LEU	4.1
1	D	560	LEU	4.1
1	F	527	LEU	4.1
1	G	409	CYS	4.1
1	I	492	LEU	4.1
1	J	145	SER	4.1
1	J	385	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
1	L	503	PHE	4.1
1	E	112	VAL	4.0
1	H	147	LYS	4.0
1	F	465	THR	4.0
1	H	107	ILE	4.0
1	L	129	ILE	4.0
1	C	414	GLY	4.0
1	D	442	GLY	4.0
1	E	329	GLY	4.0
1	A	401	SER	4.0
1	G	154	SER	4.0
1	B	321	LEU	4.0
1	H	537	LEU	4.0
1	J	514	LEU	4.0
1	A	221	LYS	4.0
1	G	512	LYS	4.0
1	H	166	ASN	4.0
1	H	229	ASN	4.0
1	I	179	ASN	4.0
1	I	303	ASN	4.0
1	D	405	ALA	4.0
1	J	553	ALA	4.0
1	B	211	VAL	4.0
1	B	551	VAL	4.0
1	G	224	VAL	4.0
1	H	207	VAL	4.0
1	I	557	VAL	4.0
1	L	206	VAL	4.0
1	L	421	VAL	4.0
1	A	263	TYR	4.0
1	A	288	TYR	4.0
1	B	115	TYR	4.0
1	G	292	TYR	4.0
1	I	423	ILE	4.0
1	G	309	SER	4.0
1	E	367	LYS	4.0
1	L	164	LYS	4.0
1	C	426	LEU	4.0
1	G	560	LEU	4.0
1	J	273	ASN	4.0
1	L	208	LEU	4.0
1	L	545	ASN	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	503	PHE	4.0
1	A	558	ALA	4.0
1	B	585	ALA	4.0
1	A	339	GLY	4.0
1	A	390	GLY	4.0
1	A	402	GLY	4.0
1	B	316	GLU	4.0
1	D	502	VAL	4.0
1	G	421	VAL	4.0
1	H	406	VAL	4.0
1	I	206	VAL	4.0
1	I	382	GLY	4.0
1	C	584	LYS	4.0
1	F	264	ILE	4.0
1	B	216	ASP	4.0
1	B	394	ASP	4.0
1	C	439	TYR	4.0
1	D	270	TYR	4.0
1	G	277	TYR	4.0
1	L	154	SER	4.0
1	C	352	ASN	4.0
1	F	505	ASN	4.0
1	B	495	LEU	4.0
1	A	289	PHE	4.0
1	H	106	PRO	4.0
1	H	441	PRO	4.0
1	H	436	LYS	4.0
1	C	372	VAL	4.0
1	D	434	VAL	4.0
1	E	190	VAL	4.0
1	L	241	THR	4.0
1	A	545	ASN	4.0
1	G	179	ASN	4.0
1	I	258	ASN	4.0
1	L	393	ILE	4.0
1	G	541	TYR	4.0
1	H	177	MET	4.0
1	C	492	LEU	4.0
1	D	234	LEU	4.0
1	D	596	LEU	4.0
1	E	310	LEU	4.0
1	E	317	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
1	G	601	LEU	4.0
1	H	470	LEU	4.0
1	H	495	LEU	4.0
1	I	596	LEU	4.0
1	H	182	LYS	4.0
1	J	523	PRO	4.0
1	L	284	ALA	4.0
1	D	398	PHE	4.0
1	A	269	VAL	4.0
1	A	520	SER	4.0
1	D	315	VAL	4.0
1	E	384	ASN	4.0
1	F	167	VAL	4.0
1	F	602	ASN	4.0
1	G	195	VAL	4.0
1	G	401	SER	4.0
1	C	513	ILE	4.0
1	E	412	CYS	4.0
1	G	271	ILE	4.0
1	B	177	MET	4.0
1	D	341	TYR	4.0
1	I	304	TYR	4.0
1	I	541	TYR	4.0
1	J	277	TYR	4.0
1	L	362	LYS	4.0
1	B	219	LEU	4.0
1	J	127	LEU	4.0
1	A	196	ALA	4.0
1	D	201	ALA	4.0
1	A	165	PHE	4.0
1	B	130	PHE	4.0
1	B	519	THR	4.0
1	D	332	GLU	4.0
1	H	262	GLU	4.0
1	A	589	LYS	4.0
1	G	406	VAL	4.0
1	H	584	LYS	4.0
1	K	344	VAL	4.0
1	K	481	ILE	3.9
1	A	192	CYS	3.9
1	C	392	MET	3.9
1	K	412	CYS	3.9

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Mol	Chain	Res	Type	RSRZ
1	J	492	LEU	3.9
1	K	127	LEU	3.9
1	K	381	GLY	3.9
1	L	581	TRP	3.9
1	B	314	ALA	3.9
1	F	508	GLU	3.9
1	H	522	GLU	3.9
1	A	118	LYS	3.9
1	B	252	PHE	3.9
1	G	238	PHE	3.9
1	H	366	LYS	3.9
1	K	289	PHE	3.9
1	L	311	SER	3.9
1	K	269	VAL	3.9
1	L	112	VAL	3.9
1	H	443	ASP	3.9
1	C	402	GLY	3.9
1	F	280	GLU	3.9
1	J	125	GLU	3.9
1	D	480	TYR	3.9
1	B	384	ASN	3.9
1	D	317	LEU	3.9
1	E	588	PRO	3.9
1	J	234	LEU	3.9
1	K	137	LYS	3.9
1	K	533	TYR	3.9
1	H	210	LEU	3.9
1	E	485	ALA	3.9
1	I	410	ALA	3.9
1	I	485	ALA	3.9
1	K	139	ASN	3.9
1	L	388	ALA	3.9
1	G	194	SER	3.9
1	J	209	SER	3.9
1	J	458	THR	3.9
1	G	187	VAL	3.9
1	L	471	VAL	3.9
1	F	221	LYS	3.9
1	A	179	ASN	3.9
1	D	418	PRO	3.9
1	F	301	PRO	3.9
1	G	139	ASN	3.9

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Mol	Chain	Res	Type	RSRZ
1	G	272	ASN	3.9
1	G	449	ASN	3.9
1	C	246	TYR	3.9
1	C	270	TYR	3.9
1	H	493	TYR	3.9
1	B	559	SER	3.9
1	D	550	SER	3.9
1	I	549	SER	3.9
1	D	581	TRP	3.9
1	D	289	PHE	3.9
1	E	378	PHE	3.9
1	I	243	PHE	3.9
1	K	591	PHE	3.9
1	J	394	ASP	3.9
1	A	290	GLY	3.9
1	B	225	VAL	3.9
1	C	206	VAL	3.9
1	H	148	VAL	3.9
1	B	233	ASN	3.9
1	C	420	ASN	3.9
1	F	506	ASN	3.9
1	K	264	ILE	3.9
1	A	293	TYR	3.9
1	B	550	SER	3.9
1	H	487	LEU	3.9
1	I	277	TYR	3.9
1	J	86	SER	3.9
1	J	439	TYR	3.9
1	K	98	SER	3.9
1	D	443	ASP	3.9
1	G	249	ASP	3.9
1	G	483	ASP	3.9
1	H	113	GLN	3.9
1	K	468	ASP	3.9
1	L	597	THR	3.9
1	B	243	PHE	3.9
1	D	561	PHE	3.9
1	G	252	PHE	3.9
1	J	238	PHE	3.9
1	B	538	ASN	3.9
1	D	496	GLY	3.9
1	F	120	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	445	ILE	3.9
1	E	101	ILE	3.9
1	F	481	ILE	3.9
1	I	101	ILE	3.9
1	K	355	ILE	3.9
1	E	554	SER	3.9
1	E	584	LYS	3.9
1	G	386	LYS	3.9
1	H	374	LYS	3.9
1	G	318	ALA	3.9
1	H	427	SER	3.9
1	J	555	SER	3.9
1	D	208	LEU	3.9
1	J	208	LEU	3.9
1	K	464	LEU	3.9
1	A	292	TYR	3.9
1	A	472	TYR	3.9
1	F	291	THR	3.9
1	L	115	TYR	3.9
1	L	377	THR	3.9
1	L	536	THR	3.9
1	B	373	GLY	3.9
1	D	565	PHE	3.9
1	F	352	ASN	3.9
1	F	375	GLY	3.9
1	I	378	PHE	3.9
1	J	306	ASN	3.9
1	K	352	ASN	3.9
1	L	403	CYS	3.9
1	F	232	LYS	3.9
1	G	540	LYS	3.9
1	A	123	VAL	3.9
1	B	355	ILE	3.9
1	D	355	ILE	3.9
1	D	523	PRO	3.9
1	F	574	ILE	3.9
1	G	330	VAL	3.9
1	I	132	VAL	3.9
1	L	101	ILE	3.9
1	B	391	SER	3.9
1	D	548	SER	3.9
1	F	116	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
1	F	550	SER	3.9
1	E	500	ALA	3.9
1	B	426	LEU	3.9
1	D	321	LEU	3.9
1	I	509	LEU	3.9
1	C	488	THR	3.8
1	E	488	THR	3.8
1	F	241	THR	3.8
1	B	292	TYR	3.8
1	G	533	TYR	3.8
1	I	270	TYR	3.8
1	J	270	TYR	3.8
1	K	217	ASN	3.8
1	L	120	GLY	3.8
1	A	243	PHE	3.8
1	B	178	PHE	3.8
1	D	591	PHE	3.8
1	G	591	PHE	3.8
1	J	409	CYS	3.8
1	G	308	VAL	3.8
1	H	264	ILE	3.8
1	H	308	VAL	3.8
1	J	92	VAL	3.8
1	J	231	ASP	3.8
1	A	369	ILE	3.8
1	F	356	HIS	3.8
1	J	593	VAL	3.8
1	K	230	VAL	3.8
1	B	299	ALA	3.8
1	B	419	GLU	3.8
1	D	447	ALA	3.8
1	I	500	ALA	3.8
1	K	577	ALA	3.8
1	L	535	ALA	3.8
1	D	466	LEU	3.8
1	H	321	LEU	3.8
1	H	446	THR	3.8
1	I	97	THR	3.8
1	I	212	THR	3.8
1	J	217	ASN	3.8
1	K	312	ASN	3.8
1	E	375	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	J	120	GLY	3.8
1	J	381	GLY	3.8
1	A	285	ARG	3.8
1	F	594	ARG	3.8
1	H	270	TYR	3.8
1	H	463	ARG	3.8
1	J	243	PHE	3.8
1	J	354	PHE	3.8
1	A	108	HIS	3.8
1	C	155	GLU	3.8
1	C	348	SER	3.8
1	J	498	SER	3.8
1	D	123	VAL	3.8
1	B	257	LYS	3.8
1	F	430	CYS	3.8
1	G	143	LYS	3.8
1	G	571	TRP	3.8
1	H	101	ILE	3.8
1	C	314	ALA	3.8
1	D	186	ALA	3.8
1	D	433	MET	3.8
1	E	585	ALA	3.8
1	F	300	ALA	3.8
1	C	255	THR	3.8
1	E	390	GLY	3.8
1	E	415	THR	3.8
1	F	371	LEU	3.8
1	F	407	LEU	3.8
1	F	537	LEU	3.8
1	I	255	THR	3.8
1	L	601	LEU	3.8
1	I	152	GLN	3.8
1	A	341	TYR	3.8
1	A	350	TYR	3.8
1	C	189	TYR	3.8
1	E	304	TYR	3.8
1	E	394	ASP	3.8
1	G	160	GLU	3.8
1	A	135	PRO	3.8
1	I	237	PHE	3.8
1	A	230	VAL	3.8
1	A	484	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	547	ILE	3.8
1	J	271	ILE	3.8
1	K	327	ILE	3.8
1	K	530	ILE	3.8
1	L	315	VAL	3.8
1	B	381	GLY	3.8
1	D	339	GLY	3.8
1	G	294	ALA	3.8
1	H	340	ALA	3.8
1	I	318	ALA	3.8
1	I	558	ALA	3.8
1	J	572	ALA	3.8
1	K	140	GLY	3.8
1	G	155	GLU	3.8
1	G	492	LEU	3.8
1	H	267	LEU	3.8
1	I	208	LEU	3.8
1	I	569	THR	3.8
1	G	197	ASP	3.8
1	K	138	GLU	3.8
1	H	173	LYS	3.8
1	I	283	LYS	3.8
1	K	587	LYS	3.8
1	A	215	HIS	3.8
1	G	559	SER	3.8
1	G	425	PHE	3.8
1	K	237	PHE	3.8
1	K	599	PHE	3.8
1	L	235	PHE	3.8
1	L	425	PHE	3.8
1	L	591	PHE	3.8
1	C	122	ASN	3.8
1	D	104	ASN	3.8
1	E	440	ARG	3.8
1	E	574	ILE	3.8
1	F	316	GLU	3.8
1	G	444	ILE	3.8
1	G	485	ALA	3.8
1	J	144	ILE	3.8
1	J	369	ILE	3.8
1	A	331	LYS	3.8
1	C	231	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
1	K	452	THR	3.8
1	C	416	LEU	3.8
1	G	595	LEU	3.8
1	J	395	LEU	3.8
1	L	131	LEU	3.8
1	F	93	SER	3.8
1	I	494	SER	3.8
1	C	244	TYR	3.8
1	C	293	TYR	3.8
1	E	359	TYR	3.8
1	E	511	ASN	3.8
1	D	200	GLU	3.8
1	A	346	LYS	3.8
1	A	563	LYS	3.8
1	B	313	ALA	3.8
1	D	150	ASP	3.8
1	H	249	ASP	3.8
1	I	137	LYS	3.8
1	F	444	ILE	3.8
1	H	447	ALA	3.8
1	I	577	ALA	3.8
1	J	558	ALA	3.8
1	F	597	THR	3.8
1	I	452	THR	3.8
1	G	234	LEU	3.8
1	G	426	LEU	3.8
1	A	384	ASN	3.8
1	A	409	CYS	3.8
1	B	311	SER	3.8
1	C	588	PRO	3.8
1	D	432	ASN	3.8
1	D	438	SER	3.8
1	E	209	SER	3.8
1	F	163	GLU	3.8
1	G	528	PRO	3.8
1	J	254	SER	3.8
1	J	567	GLN	3.8
1	K	457	ASN	3.8
1	L	100	PRO	3.8
1	A	235	PHE	3.7
1	C	408	GLY	3.7
1	I	226	PHE	3.7

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Mol	Chain	Res	Type	RSRZ
1	I	501	GLY	3.7
1	J	565	PHE	3.7
1	B	201	ALA	3.7
1	L	370	ALA	3.7
1	A	556	ILE	3.7
1	A	579	VAL	3.7
1	B	465	THR	3.7
1	C	429	VAL	3.7
1	D	574	ILE	3.7
1	E	123	VAL	3.7
1	G	101	ILE	3.7
1	I	225	VAL	3.7
1	J	413	VAL	3.7
1	E	407	LEU	3.7
1	F	464	LEU	3.7
1	J	310	LEU	3.7
1	K	208	LEU	3.7
1	K	562	LEU	3.7
1	D	134	ASN	3.7
1	E	143	LYS	3.7
1	E	273	ASN	3.7
1	C	89	PRO	3.7
1	E	418	PRO	3.7
1	H	347	GLY	3.7
1	I	256	ASP	3.7
1	I	403	CYS	3.7
1	A	103	TYR	3.7
1	E	287	TYR	3.7
1	E	293	TYR	3.7
1	H	103	TYR	3.7
1	H	252	PHE	3.7
1	H	378	PHE	3.7
1	I	293	TYR	3.7
1	J	428	ALA	3.7
1	B	576	ILE	3.7
1	C	315	VAL	3.7
1	F	567	GLN	3.7
1	H	455	VAL	3.7
1	F	531	ASN	3.7
1	H	104	ASN	3.7
1	B	424	HIS	3.7
1	G	94	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	I	527	LEU	3.7
1	J	328	LEU	3.7
1	F	100	PRO	3.7
1	K	216	ASP	3.7
1	I	419	GLU	3.7
1	C	586	ARG	3.7
1	G	594	ARG	3.7
1	A	587	LYS	3.7
1	F	589	LYS	3.7
1	H	469	ALA	3.7
1	J	263	TYR	3.7
1	C	149	ASN	3.7
1	C	415	THR	3.7
1	C	597	THR	3.7
1	J	452	THR	3.7
1	A	91	VAL	3.7
1	E	207	VAL	3.7
1	E	427	SER	3.7
1	E	579	VAL	3.7
1	F	396	MET	3.7
1	H	550	SER	3.7
1	K	554	SER	3.7
1	L	269	VAL	3.7
1	L	502	VAL	3.7
1	E	208	LEU	3.7
1	J	419	GLU	3.7
1	K	373	GLY	3.7
1	L	382	GLY	3.7
1	G	525	TRP	3.7
1	B	289	PHE	3.7
1	C	237	PHE	3.7
1	D	352	ASN	3.7
1	C	383	TYR	3.7
1	F	299	ALA	3.7
1	I	388	ALA	3.7
1	K	293	TYR	3.7
1	L	318	ALA	3.7
1	K	465	THR	3.7
1	D	262	GLU	3.7
1	G	522	GLU	3.7
1	H	93	SER	3.7
1	K	150	ASP	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	167	VAL	3.7
1	C	195	VAL	3.7
1	D	225	VAL	3.7
1	D	396	MET	3.7
1	I	123	VAL	3.7
1	I	349	MET	3.7
1	L	91	VAL	3.7
1	L	271	ILE	3.7
1	K	301	PRO	3.7
1	B	552	LYS	3.7
1	D	222	LEU	3.7
1	F	595	LEU	3.7
1	G	193	GLY	3.7
1	I	328	LEU	3.7
1	K	310	LEU	3.7
1	E	546	GLN	3.7
1	E	155	GLU	3.7
1	I	316	GLU	3.7
1	H	216	ASP	3.7
1	I	525	TRP	3.7
1	K	102	GLU	3.7
1	C	95	ASP	3.7
1	F	274	ALA	3.7
1	A	220	SER	3.7
1	B	458	THR	3.7
1	K	378	PHE	3.7
1	H	292	TYR	3.7
1	L	493	TYR	3.7
1	L	520	SER	3.7
1	A	168	LYS	3.7
1	B	106	PRO	3.7
1	D	92	VAL	3.7
1	D	162	MET	3.7
1	F	271	ILE	3.7
1	H	547	ILE	3.7
1	I	305	CYS	3.7
1	I	412	CYS	3.7
1	F	524	VAL	3.7
1	I	286	VAL	3.7
1	I	530	ILE	3.7
1	L	429	VAL	3.7
1	A	538	ASN	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	422	GLU	3.7
1	J	95	ASP	3.7
1	A	266	HIS	3.7
1	C	199	SER	3.7
1	F	201	ALA	3.7
1	H	212	THR	3.7
1	H	452	THR	3.7
1	I	105	THR	3.7
1	L	378	PHE	3.7
1	B	541	TYR	3.7
1	C	263	TYR	3.7
1	C	288	TYR	3.7
1	E	381	GLY	3.7
1	E	480	TYR	3.7
1	I	345	GLY	3.7
1	J	126	GLY	3.7
1	J	244	TYR	3.7
1	C	481	ILE	3.7
1	C	556	ILE	3.7
1	B	155	GLU	3.6
1	D	91	VAL	3.7
1	K	203	MET	3.7
1	K	163	GLU	3.6
1	L	557	VAL	3.7
1	A	208	LEU	3.6
1	B	198	LEU	3.6
1	F	192	CYS	3.6
1	J	267	LEU	3.6
1	K	229	ASN	3.6
1	J	380	SER	3.6
1	J	548	SER	3.6
1	I	497	THR	3.6
1	J	377	THR	3.6
1	K	572	ALA	3.6
1	H	200	GLU	3.6
1	B	581	TRP	3.6
1	E	526	TRP	3.6
1	A	148	VAL	3.6
1	D	393	ILE	3.6
1	E	344	VAL	3.6
1	E	491	MET	3.6
1	F	369	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	I	129	ILE	3.6
1	C	166	ASN	3.6
1	I	143	LYS	3.6
1	B	342	LEU	3.6
1	C	234	LEU	3.6
1	E	371	LEU	3.6
1	F	385	LEU	3.6
1	L	464	LEU	3.6
1	I	430	CYS	3.6
1	B	200	GLU	3.6
1	C	209	SER	3.6
1	F	559	SER	3.6
1	H	361	SER	3.6
1	I	573	HIS	3.6
1	K	324	GLU	3.6
1	A	136	GLY	3.6
1	A	490	ALA	3.6
1	A	577	ALA	3.6
1	C	501	GLY	3.6
1	G	375	GLY	3.6
1	H	536	THR	3.6
1	L	128	THR	3.6
1	B	147	LYS	3.6
1	C	587	LYS	3.6
1	J	289	PHE	3.6
1	J	378	PHE	3.6
1	K	425	PHE	3.6
1	C	202	ASP	3.6
1	F	233	ASN	3.6
1	I	384	ASN	3.6
1	K	384	ASN	3.6
1	A	129	ILE	3.6
1	B	574	ILE	3.6
1	C	115	TYR	3.6
1	D	556	ILE	3.6
1	E	325	TYR	3.6
1	G	576	ILE	3.6
1	I	99	ILE	3.6
1	B	407	LEU	3.6
1	B	440	ARG	3.6
1	E	557	VAL	3.6
1	J	132	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	K	383	TYR	3.6
1	C	219	LEU	3.6
1	C	595	LEU	3.6
1	E	214	LEU	3.6
1	G	416	LEU	3.6
1	A	397	LYS	3.6
1	A	458	THR	3.6
1	D	248	THR	3.6
1	E	497	THR	3.6
1	F	340	ALA	3.6
1	K	170	GLY	3.6
1	A	523	PRO	3.6
1	B	96	PRO	3.6
1	D	159	ASP	3.6
1	I	231	ASP	3.6
1	K	165	PHE	3.6
1	B	262	GLU	3.6
1	C	444	ILE	3.6
1	C	484	ILE	3.6
1	F	107	ILE	3.6
1	L	228	ILE	3.6
1	D	267	LEU	3.6
1	E	234	LEU	3.6
1	E	411	TYR	3.6
1	F	359	TYR	3.6
1	I	321	LEU	3.6
1	L	593	VAL	3.6
1	G	221	LYS	3.6
1	A	348	SER	3.6
1	H	119	GLY	3.6
1	A	275	ASP	3.6
1	D	202	ASP	3.6
1	D	452	THR	3.6
1	E	231	ASP	3.6
1	E	460	ALA	3.6
1	G	468	ASP	3.6
1	I	460	ALA	3.6
1	K	460	ALA	3.6
1	K	519	THR	3.6
1	J	591	PHE	3.6
1	L	599	PHE	3.6
1	D	386	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	349	MET	3.6
1	H	544	ILE	3.6
1	I	298	ILE	3.6
1	J	544	ILE	3.6
1	A	94	LEU	3.6
1	C	142	VAL	3.6
1	C	509	LEU	3.6
1	E	426	LEU	3.6
1	H	411	TYR	3.6
1	H	514	LEU	3.6
1	I	263	TYR	3.6
1	I	413	VAL	3.6
1	A	254	SER	3.6
1	D	554	SER	3.6
1	C	170	GLY	3.6
1	C	159	ASP	3.6
1	G	87	GLU	3.6
1	L	125	GLU	3.6
1	I	597	THR	3.6
1	G	567	GLN	3.6
1	H	89	PRO	3.6
1	K	300	ALA	3.6
1	B	512	LYS	3.6
1	F	182	LYS	3.6
1	F	366	LYS	3.6
1	H	331	LYS	3.6
1	C	354	PHE	3.6
1	K	565	PHE	3.6
1	B	484	ILE	3.6
1	G	355	ILE	3.6
1	H	338	MET	3.6
1	G	269	VAL	3.6
1	G	361	SER	3.6
1	L	510	ILE	3.6
1	A	509	LEU	3.6
1	C	395	LEU	3.6
1	H	94	LEU	3.6
1	J	470	LEU	3.6
1	K	157	LEU	3.6
1	F	133	ASN	3.6
1	B	525	TRP	3.6
1	C	118	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	100	PRO	3.6
1	B	89	PRO	3.6
1	B	97	THR	3.6
1	B	291	THR	3.6
1	C	523	PRO	3.6
1	J	301	PRO	3.6
1	K	314	ALA	3.5
1	K	388	ALA	3.5
1	K	588	PRO	3.6
1	E	430	CYS	3.5
1	I	409	CYS	3.5
1	E	238	PHE	3.5
1	H	289	PHE	3.5
1	A	580	SER	3.5
1	C	361	SER	3.5
1	F	216	ASP	3.5
1	G	133	ASN	3.5
1	H	99	ILE	3.5
1	I	149	ASN	3.5
1	I	381	GLY	3.5
1	J	462	GLY	3.5
1	K	209	SER	3.5
1	B	451	LYS	3.5
1	C	260	ASN	3.5
1	C	355	ILE	3.5
1	D	129	ILE	3.5
1	E	545	ASN	3.5
1	B	515	GLN	3.5
1	F	131	LEU	3.5
1	K	317	LEU	3.5
1	K	371	LEU	3.5
1	K	421	VAL	3.5
1	L	509	LEU	3.5
1	H	341	TYR	3.5
1	I	350	TYR	3.5
1	D	597	THR	3.5
1	I	291	THR	3.5
1	K	89	PRO	3.5
1	E	422	GLU	3.5
1	F	200	GLU	3.5
1	A	420	ASN	3.5
1	B	361	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	438	SER	3.5
1	C	86	SER	3.5
1	H	391	SER	3.5
1	I	587	LYS	3.5
1	E	442	GLY	3.5
1	F	561	PHE	3.5
1	J	352	ASN	3.5
1	B	510	ILE	3.5
1	E	129	ILE	3.5
1	J	481	ILE	3.5
1	K	556	ILE	3.5
1	A	321	LEU	3.5
1	A	429	VAL	3.5
1	A	524	VAL	3.5
1	A	562	LEU	3.5
1	B	487	LEU	3.5
1	C	269	VAL	3.5
1	D	230	VAL	3.5
1	D	464	LEU	3.5
1	F	330	VAL	3.5
1	G	198	LEU	3.5
1	H	562	LEU	3.5
1	K	323	LEU	3.5
1	L	317	LEU	3.5
1	A	276	THR	3.5
1	E	270	TYR	3.5
1	G	597	THR	3.5
1	H	304	TYR	3.5
1	J	304	TYR	3.5
1	A	404	ALA	3.5
1	E	299	ALA	3.5
1	I	404	ALA	3.5
1	B	337	LYS	3.5
1	C	475	LYS	3.5
1	H	231	ASP	3.5
1	G	215	HIS	3.5
1	G	548	SER	3.5
1	G	602	ASN	3.5
1	H	435	SER	3.5
1	I	578	GLY	3.5
1	L	133	ASN	3.5
1	L	462	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	G	599	PHE	3.5
1	J	175	PHE	3.5
1	E	177	MET	3.5
1	C	317	LEU	3.5
1	G	481	ILE	3.5
1	E	403	CYS	3.5
1	F	471	VAL	3.5
1	J	211	VAL	3.5
1	B	586	ARG	3.5
1	C	536	THR	3.5
1	G	415	THR	3.5
1	H	118	LYS	3.5
1	D	404	ALA	3.5
1	K	189	TYR	3.5
1	F	306	ASN	3.5
1	K	582	ASN	3.5
1	B	120	GLY	3.5
1	I	98	SER	3.5
1	I	343	SER	3.5
1	K	329	GLY	3.5
1	A	252	PHE	3.5
1	H	265	LYS	3.5
1	K	213	MET	3.5
1	B	530	ILE	3.5
1	D	336	LEU	3.5
1	I	355	ILE	3.5
1	K	228	ILE	3.5
1	K	470	LEU	3.5
1	G	344	VAL	3.5
1	I	551	VAL	3.5
1	K	211	VAL	3.5
1	C	291	THR	3.5
1	B	553	ALA	3.5
1	A	200	GLU	3.5
1	A	325	TYR	3.5
1	D	325	TYR	3.5
1	E	138	GLU	3.5
1	F	139	ASN	3.5
1	G	217	ASN	3.5
1	A	268	GLY	3.5
1	A	501	GLY	3.5
1	B	580	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	F	363	GLY	3.5
1	F	590	GLY	3.5
1	H	580	SER	3.5
1	J	343	SER	3.5
1	H	561	PHE	3.5
1	H	591	PHE	3.5
1	I	583	PHE	3.5
1	B	99	ILE	3.5
1	C	239	LEU	3.5
1	D	271	ILE	3.5
1	G	117	ILE	3.5
1	G	556	ILE	3.5
1	H	335	GLU	3.5
1	H	369	ILE	3.5
1	K	296	GLN	3.5
1	I	155	GLU	3.5
1	J	157	LEU	3.5
1	J	393	ILE	3.5
1	L	297	LEU	3.5
1	L	369	ILE	3.5
1	B	167	VAL	3.5
1	C	465	THR	3.5
1	D	114	VAL	3.5
1	E	502	VAL	3.5
1	F	207	VAL	3.5
1	F	312	ASN	3.5
1	F	415	THR	3.5
1	G	153	VAL	3.5
1	G	190	VAL	3.5
1	I	420	ASN	3.5
1	K	276	THR	3.5
1	C	274	ALA	3.5
1	A	86	SER	3.5
1	B	293	TYR	3.5
1	B	516	SER	3.5
1	C	590	GLY	3.5
1	E	589	LYS	3.5
1	F	417	LYS	3.5
1	G	288	TYR	3.5
1	G	554	SER	3.5
1	I	295	SER	3.5
1	K	244	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	109	ASP	3.5
1	D	364	ASP	3.5
1	G	296	GLN	3.5
1	C	378	PHE	3.4
1	D	252	PHE	3.4
1	D	392	MET	3.4
1	E	599	PHE	3.4
1	F	389	PRO	3.4
1	K	243	PHE	3.4
1	K	247	MET	3.4
1	E	327	ILE	3.4
1	G	166	ASN	3.4
1	I	444	ILE	3.4
1	J	453	ILE	3.4
1	L	181	ASN	3.4
1	L	217	ASN	3.4
1	L	407	LEU	3.4
1	D	331	LYS	3.4
1	E	377	THR	3.4
1	G	458	THR	3.4
1	C	573	HIS	3.4
1	D	372	VAL	3.4
1	G	456	GLY	3.4
1	I	167	VAL	3.4
1	K	278	LYS	3.4
1	F	196	ALA	3.4
1	J	501	GLY	3.4
1	I	498	SER	3.4
1	G	439	TYR	3.4
1	K	103	TYR	3.4
1	K	499	TYR	3.4
1	L	263	TYR	3.4
1	K	459	ASP	3.4
1	C	137	LYS	3.4
1	F	158	LYS	3.4
1	G	511	ASN	3.4
1	K	584	LYS	3.4
1	L	168	LYS	3.4
1	C	491	MET	3.4
1	H	243	PHE	3.4
1	J	165	PHE	3.4
1	K	338	MET	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	212	THR	3.4
1	A	355	ILE	3.4
1	B	128	THR	3.4
1	B	215	HIS	3.4
1	D	310	LEU	3.4
1	E	110	ILE	3.4
1	G	465	THR	3.4
1	I	110	ILE	3.4
1	K	574	ILE	3.4
1	A	146	SER	3.4
1	B	187	VAL	3.4
1	B	220	SER	3.4
1	C	279	GLU	3.4
1	C	299	ALA	3.4
1	C	413	VAL	3.4
1	E	98	SER	3.4
1	E	194	SER	3.4
1	F	284	ALA	3.4
1	G	405	ALA	3.4
1	H	434	VAL	3.4
1	H	508	GLU	3.4
1	I	207	VAL	3.4
1	A	567	GLN	3.4
1	J	364	ASP	3.4
1	A	533	TYR	3.4
1	C	589	LYS	3.4
1	B	352	ASN	3.4
1	J	511	ASN	3.4
1	B	532	GLU	3.4
1	H	316	GLU	3.4
1	A	354	PHE	3.4
1	B	562	LEU	3.4
1	C	238	PHE	3.4
1	E	496	GLY	3.4
1	A	427	SER	3.4
1	C	309	SER	3.4
1	D	101	ILE	3.4
1	F	209	SER	3.4
1	F	361	SER	3.4
1	F	525	TRP	3.4
1	G	156	PHE	3.4
1	I	241	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	K	105	THR	3.4
1	G	380	SER	3.4
1	G	460	ALA	3.4
1	I	515	GLN	3.4
1	K	467	ALA	3.4
1	L	300	ALA	3.4
1	A	459	ASP	3.4
1	F	455	VAL	3.4
1	G	455	VAL	3.4
1	I	249	ASP	3.4
1	C	325	TYR	3.4
1	C	440	ARG	3.4
1	E	89	PRO	3.4
1	D	462	GLY	3.4
1	G	501	GLY	3.4
1	K	592	GLY	3.4
1	A	296	GLN	3.4
1	B	247	MET	3.4
1	E	128	THR	3.4
1	E	216	ASP	3.4
1	F	458	THR	3.4
1	A	425	PHE	3.4
1	E	235	PHE	3.4
1	G	109	ASP	3.4
1	G	247	MET	3.4
1	G	328	LEU	3.4
1	G	397	LYS	3.4
1	J	232	LYS	3.4
1	J	391	SER	3.4
1	J	417	LYS	3.4
1	L	519	THR	3.4
1	H	503	PHE	3.4
1	K	416	LEU	3.4
1	B	224	VAL	3.4
1	E	195	VAL	3.4
1	H	581	TRP	3.4
1	J	167	VAL	3.4
1	J	372	VAL	3.4
1	L	167	VAL	3.4
1	L	281	VAL	3.4
1	B	227	GLU	3.4
1	E	431	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	H	306	ASN	3.4
1	K	227	GLU	3.4
1	L	507	GLU	3.4
1	D	301	PRO	3.4
1	A	193	GLY	3.4
1	D	411	TYR	3.4
1	J	418	PRO	3.4
1	K	263	TYR	3.4
1	L	541	TYR	3.4
1	A	374	LYS	3.4
1	F	266	HIS	3.4
1	J	424	HIS	3.4
1	A	171	THR	3.4
1	C	549	SER	3.4
1	F	536	THR	3.4
1	H	377	THR	3.4
1	I	520	SER	3.4
1	L	248	THR	3.4
1	C	196	ALA	3.4
1	C	271	ILE	3.4
1	D	333	LEU	3.4
1	G	192	CYS	3.4
1	I	289	PHE	3.4
1	I	416	LEU	3.4
1	K	121	CYS	3.4
1	F	566	VAL	3.4
1	L	420	ASN	3.4
1	B	182	LYS	3.4
1	K	331	LYS	3.4
1	L	113	GLN	3.4
1	E	307	PRO	3.4
1	D	231	ASP	3.4
1	F	191	GLY	3.4
1	I	590	GLY	3.4
1	A	160	GLU	3.4
1	B	555	SER	3.4
1	C	507	GLU	3.4
1	H	309	SER	3.4
1	K	439	TYR	3.4
1	A	465	THR	3.4
1	I	458	THR	3.4
1	K	458	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	149	ASN	3.4
1	A	594	ARG	3.4
1	B	186	ALA	3.4
1	B	400	MET	3.4
1	C	110	ILE	3.4
1	D	179	ASN	3.4
1	E	222	LEU	3.4
1	E	297	LEU	3.4
1	F	530	ILE	3.4
1	G	530	ILE	3.4
1	H	601	LEU	3.4
1	I	217	ASN	3.4
1	I	233	ASN	3.4
1	I	354	PHE	3.4
1	J	521	ASN	3.4
1	K	511	ASN	3.4
1	L	547	ILE	3.4
1	C	362	LYS	3.4
1	B	190	VAL	3.3
1	E	434	VAL	3.3
1	F	502	VAL	3.3
1	A	202	ASP	3.3
1	B	231	ASP	3.3
1	J	379	ASP	3.3
1	J	571	TRP	3.3
1	D	373	GLY	3.3
1	K	394	ASP	3.3
1	B	520	SER	3.3
1	C	343	SER	3.3
1	D	309	SER	3.3
1	F	86	SER	3.3
1	K	555	SER	3.3
1	L	343	SER	3.3
1	D	358	THR	3.3
1	F	497	THR	3.3
1	H	246	TYR	3.3
1	I	341	TYR	3.3
1	I	439	TYR	3.3
1	I	536	THR	3.3
1	K	497	THR	3.3
1	L	244	TYR	3.3
1	L	499	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	253	LYS	3.3
1	E	602	ASN	3.3
1	I	368	LYS	3.3
1	A	300	ALA	3.3
1	A	338	MET	3.3
1	A	370	ALA	3.3
1	C	585	ALA	3.3
1	F	410	ALA	3.3
1	E	328	LEU	3.3
1	H	90	GLN	3.3
1	D	175	PHE	3.3
1	J	117	ILE	3.3
1	A	474	GLU	3.3
1	C	419	GLU	3.3
1	F	365	VAL	3.3
1	G	114	VAL	3.3
1	G	259	VAL	3.3
1	H	402	GLY	3.3
1	K	501	GLY	3.3
1	J	573	HIS	3.3
1	A	184	SER	3.3
1	B	571	TRP	3.3
1	F	302	SER	3.3
1	F	380	SER	3.3
1	H	448	SER	3.3
1	I	571	TRP	3.3
1	K	309	SER	3.3
1	E	475	LYS	3.3
1	B	480	TYR	3.3
1	C	567	GLN	3.3
1	G	97	THR	3.3
1	G	233	ASN	3.3
1	J	465	THR	3.3
1	G	341	TYR	3.3
1	J	325	TYR	3.3
1	A	542	ALA	3.3
1	E	334	GLU	3.3
1	H	102	GLU	3.3
1	B	242	LEU	3.3
1	C	214	LEU	3.3
1	E	198	LEU	3.3
1	E	514	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	H	483	ASP	3.3
1	I	210	LEU	3.3
1	I	336	LEU	3.3
1	B	238	PHE	3.3
1	B	376	ILE	3.3
1	B	583	PHE	3.3
1	C	599	PHE	3.3
1	A	140	GLY	3.3
1	C	489	GLY	3.3
1	F	414	GLY	3.3
1	L	496	GLY	3.3
1	A	588	PRO	3.3
1	G	307	PRO	3.3
1	H	266	HIS	3.3
1	I	360	LYS	3.3
1	K	429	VAL	3.3
1	L	211	VAL	3.3
1	C	438	SER	3.3
1	F	311	SER	3.3
1	H	517	SER	3.3
1	C	133	ASN	3.3
1	H	506	ASN	3.3
1	K	571	TRP	3.3
1	D	465	THR	3.3
1	A	186	ALA	3.3
1	A	359	TYR	3.3
1	A	411	TYR	3.3
1	B	304	TYR	3.3
1	B	542	ALA	3.3
1	C	287	TYR	3.3
1	E	95	ASP	3.3
1	H	115	TYR	3.3
1	L	292	TYR	3.3
1	H	509	LEU	3.3
1	H	527	LEU	3.3
1	L	560	LEU	3.3
1	B	375	GLY	3.3
1	B	481	ILE	3.3
1	F	126	GLY	3.3
1	F	592	GLY	3.3
1	F	238	PHE	3.3
1	G	130	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
1	G	453	ILE	3.3
1	H	129	ILE	3.3
1	L	243	PHE	3.3
1	A	185	VAL	3.3
1	A	258	ASN	3.3
1	B	295	SER	3.3
1	C	524	VAL	3.3
1	D	365	VAL	3.3
1	D	420	ASN	3.3
1	D	506	ASN	3.3
1	E	580	SER	3.3
1	F	102	GLU	3.3
1	F	224	VAL	3.3
1	H	372	VAL	3.3
1	J	207	VAL	3.3
1	K	372	VAL	3.3
1	G	437	ASN	3.3
1	I	229	ASN	3.3
1	B	223	THR	3.3
1	B	486	THR	3.3
1	F	231	ASP	3.3
1	G	95	ASP	3.3
1	E	518	LYS	3.3
1	D	485	ALA	3.3
1	L	428	ALA	3.3
1	A	247	MET	3.3
1	E	392	MET	3.3
1	F	439	TYR	3.3
1	G	463	ARG	3.3
1	G	493	TYR	3.3
1	H	480	TYR	3.3
1	K	126	GLY	3.3
1	K	341	TYR	3.3
1	K	493	TYR	3.3
1	K	496	GLY	3.3
1	A	495	LEU	3.3
1	C	527	LEU	3.3
1	D	214	LEU	3.3
1	J	214	LEU	3.3
1	A	327	ILE	3.3
1	C	264	ILE	3.3
1	C	441	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	574	ILE	3.3
1	E	135	PRO	3.3
1	E	591	PHE	3.3
1	F	378	PHE	3.3
1	F	547	ILE	3.3
1	K	235	PHE	3.3
1	C	139	ASN	3.3
1	E	217	ASN	3.3
1	H	194	SER	3.3
1	H	209	SER	3.3
1	K	391	SER	3.3
1	D	308	VAL	3.3
1	F	225	VAL	3.3
1	F	269	VAL	3.3
1	F	413	VAL	3.3
1	E	374	LYS	3.3
1	H	379	ASP	3.3
1	I	443	ASP	3.3
1	A	284	ALA	3.3
1	A	373	GLY	3.3
1	B	428	ALA	3.3
1	C	578	GLY	3.3
1	J	370	ALA	3.3
1	H	400	MET	3.3
1	H	424	HIS	3.3
1	D	217	ASN	3.3
1	D	304	TYR	3.3
1	E	127	LEU	3.3
1	E	441	PRO	3.3
1	H	149	ASN	3.3
1	L	568	ASN	3.3
1	L	582	ASN	3.3
1	C	580	SER	3.3
1	F	98	SER	3.3
1	E	587	LYS	3.3
1	G	182	LYS	3.3
1	I	95	ASP	3.3
1	L	512	LYS	3.3
1	B	421	VAL	3.3
1	D	190	VAL	3.3
1	H	211	VAL	3.3
1	H	105	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	H	519	THR	3.3
1	E	462	GLY	3.2
1	G	408	GLY	3.2
1	H	456	GLY	3.2
1	E	473	ALA	3.2
1	A	166	ASN	3.2
1	B	104	ASN	3.2
1	H	420	ASN	3.2
1	A	351	PRO	3.2
1	B	213	MET	3.2
1	B	392	MET	3.2
1	H	253	LYS	3.2
1	J	218	LYS	3.2
1	B	493	TYR	3.2
1	B	527	LEU	3.2
1	C	480	TYR	3.2
1	D	293	TYR	3.2
1	F	309	SER	3.2
1	H	595	LEU	3.2
1	J	292	TYR	3.2
1	J	323	LEU	3.2
1	K	325	TYR	3.2
1	L	295	SER	3.2
1	L	361	SER	3.2
1	E	109	ASP	3.2
1	E	202	ASP	3.2
1	I	159	ASP	3.2
1	J	530	ILE	3.2
1	C	398	PHE	3.2
1	E	286	VAL	3.2
1	H	330	VAL	3.2
1	J	286	VAL	3.2
1	K	187	VAL	3.2
1	A	488	THR	3.2
1	C	223	THR	3.2
1	G	587	LYS	3.2
1	J	397	LYS	3.2
1	J	451	LYS	3.2
1	C	558	ALA	3.2
1	F	174	HIS	3.2
1	G	300	ALA	3.2
1	C	116	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	349	MET	3.2
1	D	380	SER	3.2
1	G	93	SER	3.2
1	K	262	GLU	3.2
1	L	109	ASP	3.2
1	B	560	LEU	3.2
1	E	527	LEU	3.2
1	K	219	LEU	3.2
1	A	244	TYR	3.2
1	B	444	ILE	3.2
1	B	533	TYR	3.2
1	D	103	TYR	3.2
1	D	288	TYR	3.2
1	I	445	ILE	3.2
1	J	383	TYR	3.2
1	J	484	ILE	3.2
1	J	499	TYR	3.2
1	L	293	TYR	3.2
1	L	439	TYR	3.2
1	L	546	GLN	3.2
1	B	429	VAL	3.2
1	B	471	VAL	3.2
1	H	518	LYS	3.2
1	I	429	VAL	3.2
1	J	475	LYS	3.2
1	G	446	THR	3.2
1	L	358	THR	3.2
1	G	303	ASN	3.2
1	L	432	ASN	3.2
1	C	443	ASP	3.2
1	D	558	ALA	3.2
1	G	314	ALA	3.2
1	K	95	ASP	3.2
1	F	96	PRO	3.2
1	G	220	SER	3.2
1	C	562	LEU	3.2
1	D	407	LEU	3.2
1	G	213	MET	3.2
1	J	560	LEU	3.2
1	K	333	LEU	3.2
1	B	129	ILE	3.2
1	B	221	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	158	LYS	3.2
1	C	350	TYR	3.2
1	F	228	ILE	3.2
1	G	327	ILE	3.2
1	I	228	ILE	3.2
1	K	253	LYS	3.2
1	F	341	TYR	3.2
1	L	376	ILE	3.2
1	C	503	PHE	3.2
1	F	403	CYS	3.2
1	J	226	PHE	3.2
1	A	408	GLY	3.2
1	E	413	VAL	3.2
1	E	455	VAL	3.2
1	F	104	ASN	3.2
1	H	282	GLU	3.2
1	I	227	GLU	3.2
1	I	602	ASN	3.2
1	A	424	HIS	3.2
1	A	141	PRO	3.2
1	B	435	SER	3.2
1	C	184	SER	3.2
1	F	295	SER	3.2
1	I	184	SER	3.2
1	I	588	PRO	3.2
1	G	546	GLN	3.2
1	C	560	LEU	3.2
1	K	537	LEU	3.2
1	B	264	ILE	3.2
1	B	327	ILE	3.2
1	H	408	GLY	3.2
1	L	327	ILE	3.2
1	A	304	TYR	3.2
1	A	449	ASN	3.2
1	E	244	TYR	3.2
1	F	503	PHE	3.2
1	H	235	PHE	3.2
1	I	503	PHE	3.2
1	J	103	TYR	3.2
1	J	130	PHE	3.2
1	J	526	TRP	3.2
1	K	545	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	519	THR	3.2
1	C	114	VAL	3.2
1	C	593	VAL	3.2
1	D	536	THR	3.2
1	G	225	VAL	3.2
1	J	97	THR	3.2
1	J	248	THR	3.2
1	L	458	THR	3.2
1	A	451	LYS	3.2
1	C	388	ALA	3.2
1	C	447	ALA	3.2
1	C	467	ALA	3.2
1	F	460	ALA	3.2
1	I	564	GLU	3.2
1	J	213	MET	3.2
1	K	214	LEU	3.2
1	C	382	GLY	3.2
1	C	568	ASN	3.2
1	D	345	GLY	3.2
1	H	272	ASN	3.2
1	D	379	ASP	3.2
1	F	453	ILE	3.2
1	J	107	ILE	3.2
1	K	544	ILE	3.2
1	B	499	TYR	3.2
1	C	289	PHE	3.2
1	G	563	LYS	3.2
1	I	326	LYS	3.2
1	J	398	PHE	3.2
1	K	174	HIS	3.2
1	K	204	LYS	3.2
1	A	187	VAL	3.2
1	C	546	GLN	3.2
1	E	482	VAL	3.2
1	E	566	VAL	3.2
1	A	102	GLU	3.2
1	C	412	CYS	3.2
1	F	220	SER	3.2
1	H	507	GLU	3.2
1	A	570	ALA	3.2
1	F	351	PRO	3.2
1	L	196	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	437	ASN	3.2
1	D	602	ASN	3.2
1	E	104	ASN	3.2
1	B	218	LYS	3.2
1	B	596	LEU	3.2
1	C	242	LEU	3.2
1	F	339	GLY	3.2
1	G	168	LYS	3.2
1	K	198	LEU	3.2
1	L	416	LEU	3.2
1	A	155	GLU	3.1
1	A	529	ILE	3.1
1	A	497	THR	3.1
1	E	200	GLU	3.1
1	F	335	GLU	3.1
1	G	445	ILE	3.1
1	G	510	ILE	3.1
1	H	241	THR	3.1
1	L	105	THR	3.1
1	L	124	GLU	3.1
1	D	263	TYR	3.1
1	F	175	PHE	3.1
1	B	427	SER	3.1
1	F	244	TYR	3.1
1	H	533	TYR	3.1
1	K	270	TYR	3.1
1	J	524	VAL	3.1
1	K	199	SER	3.1
1	L	325	TYR	3.1
1	C	112	VAL	3.1
1	H	471	VAL	3.1
1	C	571	TRP	3.1
1	J	525	TRP	3.1
1	D	299	ALA	3.1
1	E	186	ALA	3.1
1	L	447	ALA	3.1
1	A	306	ASN	3.1
1	D	278	LYS	3.1
1	F	205	ARG	3.1
1	F	603	ASP	3.1
1	H	320	LYS	3.1
1	J	149	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	363	GLY	3.1
1	J	119	GLY	3.1
1	C	222	LEU	3.1
1	F	515	GLN	3.1
1	C	358	THR	3.1
1	G	486	THR	3.1
1	H	291	THR	3.1
1	J	444	ILE	3.1
1	J	597	THR	3.1
1	K	144	ILE	3.1
1	K	513	ILE	3.1
1	E	165	PHE	3.1
1	E	561	PHE	3.1
1	F	591	PHE	3.1
1	H	311	SER	3.1
1	K	548	SER	3.1
1	A	307	PRO	3.1
1	B	246	TYR	3.1
1	C	455	VAL	3.1
1	D	588	PRO	3.1
1	E	91	VAL	3.1
1	E	103	TYR	3.1
1	F	307	PRO	3.1
1	K	512	LYS	3.1
1	H	294	ALA	3.1
1	A	245	GLU	3.1
1	E	324	GLU	3.1
1	F	160	GLU	3.1
1	H	430	CYS	3.1
1	A	317	LEU	3.1
1	B	239	LEU	3.1
1	E	509	LEU	3.1
1	F	416	LEU	3.1
1	K	349	MET	3.1
1	L	349	MET	3.1
1	F	285	ARG	3.1
1	F	513	ILE	3.1
1	G	204	LYS	3.1
1	I	362	LYS	3.1
1	J	554	SER	3.1
1	K	368	LYS	3.1
1	K	445	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	237	PHE	3.1
1	G	531	ASN	3.1
1	I	106	PRO	3.1
1	J	237	PHE	3.1
1	K	133	ASN	3.1
1	K	461	GLU	3.1
1	K	505	ASN	3.1
1	A	344	VAL	3.1
1	C	201	ALA	3.1
1	G	281	VAL	3.1
1	I	383	TYR	3.1
1	K	359	TYR	3.1
1	K	546	GLN	3.1
1	L	500	ALA	3.1
1	D	489	GLY	3.1
1	G	140	GLY	3.1
1	G	339	GLY	3.1
1	L	345	GLY	3.1
1	L	356	HIS	3.1
1	K	143	LYS	3.1
1	C	203	MET	3.1
1	C	342	LEU	3.1
1	E	192	CYS	3.1
1	F	476	LEU	3.1
1	F	495	LEU	3.1
1	G	208	LEU	3.1
1	A	309	SER	3.1
1	I	440	ARG	3.1
1	K	516	SER	3.1
1	A	468	ASP	3.1
1	D	105	THR	3.1
1	L	97	THR	3.1
1	L	212	THR	3.1
1	B	449	ASN	3.1
1	H	531	ASN	3.1
1	I	453	ILE	3.1
1	C	301	PRO	3.1
1	L	306	ASN	3.1
1	F	243	PHE	3.1
1	H	583	PHE	3.1
1	A	410	ALA	3.1
1	B	406	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	542	ALA	3.1
1	E	170	GLY	3.1
1	F	387	ALA	3.1
1	G	274	ALA	3.1
1	G	590	GLY	3.1
1	I	91	VAL	3.1
1	K	186	ALA	3.1
1	E	288	TYR	3.1
1	E	499	TYR	3.1
1	F	325	TYR	3.1
1	D	111	LYS	3.1
1	I	356	HIS	3.1
1	K	205	ARG	3.1
1	B	448	SER	3.1
1	C	596	LEU	3.1
1	D	145	SER	3.1
1	D	575	ASP	3.1
1	E	157	LEU	3.1
1	E	323	LEU	3.1
1	E	342	LEU	3.1
1	E	539	SER	3.1
1	G	466	LEU	3.1
1	I	127	LEU	3.1
1	I	470	LEU	3.1
1	J	338	MET	3.1
1	J	562	LEU	3.1
1	E	133	ASN	3.1
1	E	241	THR	3.1
1	G	161	ASN	3.1
1	G	181	ASN	3.1
1	G	519	THR	3.1
1	G	545	ASN	3.1
1	I	128	THR	3.1
1	B	305	CYS	3.1
1	E	228	ILE	3.1
1	G	99	ILE	3.1
1	H	298	ILE	3.1
1	A	436	LYS	3.1
1	B	570	ALA	3.1
1	C	130	PHE	3.1
1	E	540	LYS	3.1
1	J	382	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	K	402	GLY	3.1
1	C	300	ALA	3.1
1	A	315	VAL	3.1
1	D	281	VAL	3.1
1	D	600	VAL	3.1
1	E	315	VAL	3.1
1	G	200	GLU	3.1
1	H	142	VAL	3.1
1	H	557	VAL	3.1
1	I	185	VAL	3.1
1	D	350	TYR	3.1
1	E	586	ARG	3.1
1	A	231	ASP	3.1
1	E	364	ASP	3.1
1	A	122	ASN	3.1
1	B	209	SER	3.1
1	C	98	SER	3.1
1	H	312	ASN	3.1
1	I	554	SER	3.1
1	A	371	LEU	3.1
1	A	525	TRP	3.1
1	J	420	ASN	3.1
1	D	509	LEU	3.1
1	E	536	THR	3.1
1	F	214	LEU	3.1
1	J	291	THR	3.1
1	J	342	LEU	3.1
1	C	218	LYS	3.1
1	I	337	LYS	3.1
1	K	241	THR	3.1
1	K	386	LYS	3.1
1	K	569	THR	3.1
1	L	89	PRO	3.1
1	A	462	GLY	3.1
1	B	423	ILE	3.1
1	D	381	GLY	3.1
1	D	532	GLU	3.1
1	D	590	GLY	3.1
1	H	363	GLY	3.1
1	H	461	GLU	3.1
1	K	129	ILE	3.1
1	K	290	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	G	410	ALA	3.1
1	G	553	ALA	3.1
1	J	577	ALA	3.1
1	K	561	PHE	3.1
1	L	586	ARG	3.1
1	F	215	HIS	3.0
1	A	493	TYR	3.0
1	I	493	TYR	3.0
1	J	533	TYR	3.0
1	K	176	TYR	3.0
1	A	582	ASN	3.0
1	B	360	LYS	3.0
1	I	309	SER	3.0
1	J	360	LYS	3.0
1	B	102	GLU	3.0
1	B	601	LEU	3.0
1	E	162	MET	3.0
1	G	124	GLU	3.0
1	K	342	LEU	3.0
1	K	476	LEU	3.0
1	E	402	GLY	3.0
1	E	571	TRP	3.0
1	I	89	PRO	3.0
1	I	418	PRO	3.0
1	D	530	ILE	3.0
1	E	529	ILE	3.0
1	H	376	ILE	3.0
1	I	544	ILE	3.0
1	I	574	ILE	3.0
1	L	481	ILE	3.0
1	A	394	ASP	3.0
1	C	318	ALA	3.0
1	D	275	ASP	3.0
1	D	388	ALA	3.0
1	E	313	ALA	3.0
1	F	399	ASP	3.0
1	J	485	ALA	3.0
1	L	430	CYS	3.0
1	A	540	LYS	3.0
1	H	218	LYS	3.0
1	E	166	ASN	3.0
1	G	432	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	G	505	ASN	3.0
1	H	315	VAL	3.0
1	I	269	VAL	3.0
1	A	332	GLU	3.0
1	A	559	SER	3.0
1	C	427	SER	3.0
1	C	554	SER	3.0
1	D	189	TYR	3.0
1	D	246	TYR	3.0
1	D	539	SER	3.0
1	E	341	TYR	3.0
1	G	348	SER	3.0
1	K	472	TYR	3.0
1	A	169	LEU	3.0
1	B	466	LEU	3.0
1	B	537	LEU	3.0
1	B	578	GLY	3.0
1	C	241	THR	3.0
1	D	477	GLY	3.0
1	I	297	LEU	3.0
1	K	377	THR	3.0
1	A	113	GLN	3.0
1	A	386	LYS	3.0
1	A	481	ILE	3.0
1	B	469	ALA	3.0
1	C	215	HIS	3.0
1	C	544	ILE	3.0
1	F	173	LYS	3.0
1	F	318	ALA	3.0
1	F	370	ALA	3.0
1	H	481	ILE	3.0
1	K	294	ALA	3.0
1	C	316	GLU	3.0
1	D	139	ASN	3.0
1	E	87	GLU	3.0
1	J	422	GLU	3.0
1	C	448	SER	3.0
1	F	494	SER	3.0
1	F	586	ARG	3.0
1	H	541	TYR	3.0
1	I	594	ARG	3.0
1	K	411	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	382	GLY	3.0
1	C	345	GLY	3.0
1	I	290	GLY	3.0
1	D	135	PRO	3.0
1	E	358	THR	3.0
1	E	452	THR	3.0
1	C	366	LYS	3.0
1	F	357	LEU	3.0
1	G	177	MET	3.0
1	L	396	MET	3.0
1	K	474	GLU	3.0
1	A	573	HIS	3.0
1	A	352	ASN	3.0
1	C	369	ILE	3.0
1	C	485	ALA	3.0
1	D	181	ASN	3.0
1	E	303	ASN	3.0
1	F	393	ILE	3.0
1	G	306	ASN	3.0
1	G	542	ALA	3.0
1	I	352	ASN	3.0
1	I	521	ASN	3.0
1	K	542	ALA	3.0
1	L	272	ASN	3.0
1	L	530	ILE	3.0
1	C	498	SER	3.0
1	E	243	PHE	3.0
1	J	494	SER	3.0
1	K	236	ARG	3.0
1	L	354	PHE	3.0
1	F	308	VAL	3.0
1	C	191	GLY	3.0
1	C	386	LYS	3.0
1	H	375	GLY	3.0
1	A	441	PRO	3.0
1	B	103	TYR	3.0
1	C	515	GLN	3.0
1	D	292	TYR	3.0
1	E	335	GLU	3.0
1	G	113	GLN	3.0
1	G	379	ASP	3.0
1	H	95	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	H	288	TYR	3.0
1	I	480	TYR	3.0
1	K	141	PRO	3.0
1	D	131	LEU	3.0
1	E	476	LEU	3.0
1	F	349	MET	3.0
1	I	177	MET	3.0
1	B	356	HIS	3.0
1	C	582	ASN	3.0
1	D	573	HIS	3.0
1	K	531	ASN	3.0
1	F	251	ARG	3.0
1	F	469	ALA	3.0
1	G	196	ALA	3.0
1	J	340	ALA	3.0
1	A	548	SER	3.0
1	A	555	SER	3.0
1	C	520	SER	3.0
1	E	220	SER	3.0
1	K	107	ILE	3.0
1	L	93	SER	3.0
1	B	584	LYS	3.0
1	C	283	LYS	3.0
1	F	204	LYS	3.0
1	G	584	LYS	3.0
1	J	337	LYS	3.0
1	H	332	GLU	3.0
1	I	178	PHE	3.0
1	I	522	GLU	3.0
1	J	252	PHE	3.0
1	J	344	VAL	3.0
1	K	120	GLY	3.0
1	F	109	ASP	3.0
1	G	399	ASP	3.0
1	K	413	VAL	3.0
1	K	483	ASP	3.0
1	K	543	ASP	3.0
1	L	185	VAL	3.0
1	C	100	PRO	3.0
1	G	452	THR	3.0
1	C	277	TYR	3.0
1	E	263	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
1	F	480	TYR	3.0
1	G	573	HIS	3.0
1	I	511	ASN	3.0
1	J	321	LEU	3.0
1	J	464	LEU	3.0
1	K	239	LEU	3.0
1	C	594	ARG	3.0
1	J	440	ARG	3.0
1	A	138	GLU	3.0
1	B	522	GLU	3.0
1	H	570	ALA	3.0
1	I	380	SER	3.0
1	I	405	ALA	3.0
1	J	294	ALA	3.0
1	D	99	ILE	3.0
1	E	107	ILE	3.0
1	B	249	ASP	3.0
1	G	394	ASP	3.0
1	G	496	GLY	3.0
1	F	165	PHE	3.0
1	F	526	TRP	3.0
1	I	307	PRO	3.0
1	C	104	ASN	3.0
1	C	306	ASN	3.0
1	I	166	ASN	3.0
1	J	486	THR	3.0
1	K	322	ASN	3.0
1	B	278	LYS	3.0
1	F	283	LYS	3.0
1	G	108	HIS	3.0
1	J	205	ARG	3.0
1	C	341	TYR	2.9
1	D	342	LEU	2.9
1	D	359	TYR	2.9
1	F	338	MET	2.9
1	H	222	LEU	2.9
1	L	385	LEU	2.9
1	C	430	CYS	2.9
1	A	516	SER	2.9
1	B	254	SER	2.9
1	B	284	ALA	2.9
1	L	467	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	543	ASP	2.9
1	F	275	ASP	2.9
1	I	575	ASP	2.9
1	J	483	ASP	2.9
1	A	101	ILE	2.9
1	B	191	GLY	2.9
1	A	238	PHE	2.9
1	E	346	LYS	2.9
1	K	226	PHE	2.9
1	C	225	VAL	2.9
1	E	432	ASN	2.9
1	H	526	TRP	2.9
1	I	322	ASN	2.9
1	D	280	GLU	2.9
1	A	438	SER	2.9
1	C	433	MET	2.9
1	D	435	SER	2.9
1	D	491	MET	2.9
1	E	242	LEU	2.9
1	G	157	LEU	2.9
1	G	210	LEU	2.9
1	I	323	LEU	2.9
1	E	145	SER	2.9
1	F	555	SER	2.9
1	I	325	TYR	2.9
1	I	361	SER	2.9
1	J	541	TYR	2.9
1	K	231	ASP	2.9
1	B	490	ALA	2.9
1	G	388	ALA	2.9
1	L	570	ALA	2.9
1	A	590	GLY	2.9
1	D	456	GLY	2.9
1	F	381	GLY	2.9
1	H	329	GLY	2.9
1	L	477	GLY	2.9
1	C	278	LYS	2.9
1	L	423	ILE	2.9
1	A	124	GLU	2.9
1	B	334	GLU	2.9
1	G	586	ARG	2.9
1	C	432	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	J	181	ASN	2.9
1	A	106	PRO	2.9
1	I	301	PRO	2.9
1	G	223	THR	2.9
1	J	206	VAL	2.9
1	K	212	THR	2.9
1	L	92	VAL	2.9
1	A	479	ASP	2.9
1	B	399	ASP	2.9
1	C	379	ASP	2.9
1	D	109	ASP	2.9
1	E	468	ASP	2.9
1	F	249	ASP	2.9
1	J	180	ASP	2.9
1	B	343	SER	2.9
1	H	208	LEU	2.9
1	J	220	SER	2.9
1	K	514	LEU	2.9
1	L	554	SER	2.9
1	C	473	ALA	2.9
1	D	533	TYR	2.9
1	J	137	LYS	2.9
1	J	143	LYS	2.9
1	L	368	LYS	2.9
1	F	490	ALA	2.9
1	G	332	GLU	2.9
1	I	375	GLY	2.9
1	J	329	GLY	2.9
1	B	420	ASN	2.9
1	E	481	ILE	2.9
1	C	178	PHE	2.9
1	J	519	THR	2.9
1	K	252	PHE	2.9
1	K	446	THR	2.9
1	D	132	VAL	2.9
1	F	92	VAL	2.9
1	G	231	ASP	2.9
1	I	142	VAL	2.9
1	G	367	LYS	2.9
1	H	563	LYS	2.9
1	D	571	TRP	2.9
1	E	240	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	G	598	GLU	2.9
1	J	154	SER	2.9
1	K	86	SER	2.9
1	K	448	SER	2.9
1	L	200	GLU	2.9
1	L	279	GLU	2.9
1	A	120	GLY	2.9
1	A	131	LEU	2.9
1	A	416	LEU	2.9
1	B	509	LEU	2.9
1	C	396	MET	2.9
1	G	170	GLY	2.9
1	H	491	MET	2.9
1	I	402	GLY	2.9
1	J	193	GLY	2.9
1	J	203	MET	2.9
1	J	416	LEU	2.9
1	C	370	ALA	2.9
1	D	115	TYR	2.9
1	E	572	ALA	2.9
1	D	384	ASN	2.9
1	F	350	TYR	2.9
1	G	287	TYR	2.9
1	I	313	ALA	2.9
1	L	553	ALA	2.9
1	L	273	ASN	2.9
1	C	101	ILE	2.9
1	C	445	ILE	2.9
1	D	144	ILE	2.9
1	D	510	ILE	2.9
1	K	444	ILE	2.9
1	D	116	ASP	2.9
1	J	197	ASP	2.9
1	J	128	THR	2.9
1	A	178	PHE	2.9
1	B	591	PHE	2.9
1	E	252	PHE	2.9
1	A	554	SER	2.9
1	B	413	VAL	2.9
1	C	281	VAL	2.9
1	E	185	VAL	2.9
1	F	391	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	G	207	VAL	2.9
1	J	365	VAL	2.9
1	L	555	SER	2.9
1	C	476	LEU	2.9
1	D	357	LEU	2.9
1	D	371	LEU	2.9
1	F	222	LEU	2.9
1	J	198	LEU	2.9
1	F	428	ALA	2.9
1	F	467	ALA	2.9
1	G	313	ALA	2.9
1	L	433	MET	2.9
1	F	353	LYS	2.9
1	F	451	LYS	2.9
1	J	147	LYS	2.9
1	J	341	TYR	2.9
1	C	266	HIS	2.9
1	E	573	HIS	2.9
1	G	441	PRO	2.9
1	H	575	ASP	2.9
1	K	351	PRO	2.9
1	K	424	HIS	2.9
1	J	355	ILE	2.9
1	C	105	THR	2.9
1	E	463	ARG	2.9
1	G	440	ARG	2.9
1	I	223	THR	2.9
1	L	205	ARG	2.9
1	H	555	SER	2.9
1	G	403	CYS	2.9
1	G	430	CYS	2.9
1	I	235	PHE	2.9
1	L	559	SER	2.9
1	C	566	VAL	2.9
1	D	593	VAL	2.9
1	F	132	VAL	2.9
1	H	188	GLY	2.9
1	K	600	VAL	2.9
1	L	413	VAL	2.9
1	A	273	ASN	2.9
1	D	545	ASN	2.9
1	G	183	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	G	506	ASN	2.9
1	C	374	LYS	2.9
1	C	262	GLU	2.9
1	C	522	GLU	2.9
1	D	335	GLU	2.9
1	D	340	ALA	2.9
1	E	267	LEU	2.9
1	E	400	MET	2.9
1	I	239	LEU	2.9
1	I	433	MET	2.9
1	L	102	GLU	2.9
1	F	95	ASP	2.9
1	H	525	TRP	2.9
1	G	270	TYR	2.9
1	J	89	PRO	2.9
1	D	298	ILE	2.8
1	D	529	ILE	2.8
1	H	576	ILE	2.8
1	J	510	ILE	2.8
1	K	271	ILE	2.8
1	A	128	THR	2.8
1	A	241	THR	2.8
1	G	448	SER	2.8
1	L	516	SER	2.8
1	B	152	GLN	2.8
1	G	538	ASN	2.8
1	K	456	GLY	2.8
1	B	503	PHE	2.8
1	C	226	PHE	2.8
1	D	583	PHE	2.8
1	I	257	LYS	2.8
1	E	132	VAL	2.8
1	G	125	GLU	2.8
1	H	250	GLU	2.8
1	K	279	GLU	2.8
1	K	403	CYS	2.8
1	B	349	MET	2.8
1	B	387	ALA	2.8
1	E	542	ALA	2.8
1	G	495	LEU	2.8
1	I	491	MET	2.8
1	J	131	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	J	601	LEU	2.8
1	L	405	ALA	2.8
1	L	585	ALA	2.8
1	B	463	ARG	2.8
1	F	411	TYR	2.8
1	A	151	LYS	2.8
1	B	461	GLU	2.8
1	C	128	THR	2.8
1	D	291	THR	2.8
1	D	444	ILE	2.8
1	D	518	LYS	2.8
1	G	241	THR	2.8
1	G	423	ILE	2.8
1	I	529	ILE	2.8
1	H	268	GLY	2.8
1	H	295	SER	2.8
1	J	559	SER	2.8
1	K	172	SER	2.8
1	L	118	LYS	2.8
1	F	390	GLY	2.8
1	F	598	GLU	2.8
1	G	420	ASN	2.8
1	C	190	VAL	2.8
1	D	406	VAL	2.8
1	D	566	VAL	2.8
1	E	379	ASP	2.8
1	G	88	VAL	2.8
1	I	482	VAL	2.8
1	B	285	ARG	2.8
1	A	492	LEU	2.8
1	B	485	ALA	2.8
1	C	328	LEU	2.8
1	D	527	LEU	2.8
1	E	388	ALA	2.8
1	E	447	ALA	2.8
1	I	186	ALA	2.8
1	J	407	LEU	2.8
1	L	404	ALA	2.8
1	L	305	CYS	2.8
1	E	360	LYS	2.8
1	J	278	LYS	2.8
1	L	523	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	L	332	GLU	2.8
1	B	113	GLN	2.8
1	B	348	SER	2.8
1	C	531	ASN	2.8
1	E	183	ASN	2.8
1	F	498	SER	2.8
1	H	590	GLY	2.8
1	I	246	TYR	2.8
1	I	348	SER	2.8
1	I	359	TYR	2.8
1	J	188	GLY	2.8
1	J	581	TRP	2.8
1	K	292	TYR	2.8
1	L	98	SER	2.8
1	L	402	GLY	2.8
1	L	435	SER	2.8
1	L	549	SER	2.8
1	E	212	THR	2.8
1	E	248	THR	2.8
1	F	105	THR	2.8
1	K	453	ILE	2.8
1	A	226	PHE	2.8
1	J	503	PHE	2.8
1	B	344	VAL	2.8
1	I	471	VAL	2.8
1	K	286	VAL	2.8
1	E	124	GLU	2.8
1	I	570	ALA	2.8
1	G	321	LEU	2.8
1	H	407	LEU	2.8
1	I	113	GLN	2.8
1	K	433	MET	2.8
1	L	400	MET	2.8
1	C	521	ASN	2.8
1	F	384	ASN	2.8
1	G	568	ASN	2.8
1	J	449	ASN	2.8
1	C	375	GLY	2.8
1	C	401	SER	2.8
1	C	559	SER	2.8
1	E	268	GLY	2.8
1	H	290	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	L	194	SER	2.8
1	L	375	GLY	2.8
1	B	287	TYR	2.8
1	D	287	TYR	2.8
1	D	499	TYR	2.8
1	J	423	ILE	2.8
1	D	226	PHE	2.8
1	D	354	PHE	2.8
1	C	92	VAL	2.8
1	G	429	VAL	2.8
1	D	553	ALA	2.8
1	E	428	ALA	2.8
1	H	299	ALA	2.8
1	A	505	ASN	2.8
1	B	214	LEU	2.8
1	C	169	LEU	2.8
1	D	441	PRO	2.8
1	H	426	LEU	2.8
1	H	505	ASN	2.8
1	L	384	ASN	2.8
1	L	538	ASN	2.8
1	G	98	SER	2.8
1	G	504	GLY	2.8
1	I	401	SER	2.8
1	L	590	GLY	2.8
1	A	586	ARG	2.8
1	L	575	ASP	2.8
1	B	507	GLU	2.8
1	C	368	LYS	2.8
1	J	564	GLU	2.8
1	L	262	GLU	2.8
1	C	176	TYR	2.8
1	I	176	TYR	2.8
1	J	359	TYR	2.8
1	K	304	TYR	2.8
1	L	304	TYR	2.8
1	L	152	GLN	2.8
1	F	108	HIS	2.8
1	B	303	ASN	2.8
1	D	322	ASN	2.8
1	D	351	PRO	2.8
1	D	473	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	538	ASN	2.8
1	G	165	PHE	2.8
1	F	89	PRO	2.8
1	J	314	ALA	2.8
1	J	318	ALA	2.8
1	K	123	VAL	2.8
1	L	96	PRO	2.8
1	L	201	ALA	2.8
1	B	94	LEU	2.8
1	H	86	SER	2.8
1	H	401	SER	2.8
1	I	164	LYS	2.8
1	J	204	LYS	2.8
1	L	316	GLU	2.8
1	C	377	THR	2.8
1	K	430	CYS	2.8
1	K	529	ILE	2.8
1	A	499	TYR	2.8
1	G	103	TYR	2.8
1	J	350	TYR	2.8
1	A	312	ASN	2.8
1	C	233	ASN	2.8
1	D	183	ASN	2.8
1	E	149	ASN	2.8
1	G	122	ASN	2.8
1	H	545	ASN	2.8
1	I	531	ASN	2.8
1	B	138	GLU	2.8
1	B	386	LYS	2.8
1	D	205	ARG	2.8
1	F	334	GLU	2.8
1	G	299	ALA	2.7
1	G	507	GLU	2.8
1	J	124	GLU	2.8
1	J	362	LYS	2.8
1	J	587	LYS	2.8
1	D	142	VAL	2.7
1	E	175	PHE	2.7
1	J	566	VAL	2.7
1	K	404	ALA	2.7
1	K	431	GLU	2.8
1	A	98	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	329	GLY	2.7
1	H	482	VAL	2.7
1	I	190	VAL	2.7
1	G	539	SER	2.7
1	I	390	GLY	2.7
1	J	172	SER	2.7
1	J	347	GLY	2.7
1	J	502	VAL	2.7
1	F	401	SER	2.7
1	I	391	SER	2.7
1	K	145	SER	2.7
1	L	184	SER	2.7
1	B	470	LEU	2.7
1	C	336	LEU	2.7
1	F	392	MET	2.7
1	G	333	LEU	2.7
1	L	392	MET	2.7
1	D	296	GLN	2.7
1	L	567	GLN	2.7
1	A	97	THR	2.7
1	B	212	THR	2.7
1	B	452	THR	2.7
1	B	497	THR	2.7
1	E	105	THR	2.7
1	I	486	THR	2.7
1	B	87	GLU	2.7
1	B	160	GLU	2.7
1	B	474	GLU	2.7
1	C	174	HIS	2.7
1	C	179	ASN	2.7
1	C	449	ASN	2.7
1	C	530	ILE	2.7
1	D	102	GLU	2.7
1	D	360	LYS	2.7
1	I	139	ASN	2.7
1	I	508	GLU	2.7
1	K	552	LYS	2.7
1	D	463	ARG	2.7
1	A	121	CYS	2.7
1	A	270	TYR	2.7
1	H	543	ASP	2.7
1	L	479	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	126	GLY	2.7
1	A	450	GLY	2.7
1	B	526	TRP	2.7
1	D	290	GLY	2.7
1	D	370	ALA	2.7
1	E	467	ALA	2.7
1	E	477	GLY	2.7
1	H	467	ALA	2.7
1	J	339	GLY	2.7
1	C	600	VAL	2.7
1	E	167	VAL	2.7
1	F	226	PHE	2.7
1	I	559	SER	2.7
1	E	296	GLN	2.7
1	I	112	VAL	2.7
1	F	333	LEU	2.7
1	I	219	LEU	2.7
1	L	328	LEU	2.7
1	H	415	THR	2.7
1	C	217	ASN	2.7
1	D	161	ASN	2.7
1	I	568	ASN	2.7
1	L	233	ASN	2.7
1	I	116	ASP	2.7
1	F	510	ILE	2.7
1	J	327	ILE	2.7
1	B	100	PRO	2.7
1	F	408	GLY	2.7
1	F	348	SER	2.7
1	H	359	TYR	2.7
1	A	190	VAL	2.7
1	B	434	VAL	2.7
1	C	425	PHE	2.7
1	D	526	TRP	2.7
1	E	227	GLU	2.7
1	G	230	VAL	2.7
1	G	374	LYS	2.7
1	J	153	VAL	2.7
1	D	595	LEU	2.7
1	I	400	MET	2.7
1	E	597	THR	2.7
1	G	377	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	95	ASP	2.7
1	E	424	HIS	2.7
1	E	483	ASP	2.7
1	F	511	ASN	2.7
1	F	545	ASN	2.7
1	E	501	GLY	2.7
1	L	456	GLY	2.7
1	C	96	PRO	2.7
1	A	283	LYS	2.7
1	B	250	GLU	2.7
1	H	124	GLU	2.7
1	I	232	LYS	2.7
1	I	540	LYS	2.7
1	K	87	GLU	2.7
1	K	508	GLU	2.7
1	L	160	GLU	2.7
1	B	383	TYR	2.7
1	C	304	TYR	2.7
1	G	293	TYR	2.7
1	G	359	TYR	2.7
1	G	572	ALA	2.7
1	K	350	TYR	2.7
1	K	387	ALA	2.7
1	C	421	VAL	2.7
1	D	130	PHE	2.7
1	H	593	VAL	2.7
1	H	600	VAL	2.7
1	I	600	VAL	2.7
1	J	463	ARG	2.7
1	K	178	PHE	2.7
1	A	213	MET	2.7
1	A	432	ASN	2.7
1	B	358	THR	2.7
1	B	377	THR	2.7
1	B	415	THR	2.7
1	B	506	ASN	2.7
1	E	321	LEU	2.7
1	D	483	ASP	2.7
1	E	525	TRP	2.7
1	G	384	ASN	2.7
1	I	519	THR	2.7
1	K	171	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	L	497	THR	2.7
1	C	125	GLU	2.7
1	G	290	GLY	2.7
1	J	592	GLY	2.7
1	K	462	GLY	2.7
1	D	580	SER	2.7
1	H	307	PRO	2.7
1	K	110	ILE	2.7
1	B	473	ALA	2.7
1	D	585	ALA	2.7
1	F	500	ALA	2.7
1	G	370	ALA	2.7
1	G	428	ALA	2.7
1	H	577	ALA	2.7
1	F	541	TYR	2.7
1	G	411	TYR	2.7
1	G	459	ASP	2.7
1	E	178	PHE	2.7
1	G	226	PHE	2.7
1	G	237	PHE	2.7
1	J	457	ASN	2.7
1	H	286	VAL	2.7
1	G	497	THR	2.7
1	I	222	LEU	2.7
1	J	242	LEU	2.7
1	K	167	VAL	2.7
1	E	174	HIS	2.7
1	K	527	LEU	2.7
1	B	151	LYS	2.7
1	E	564	GLU	2.7
1	G	353	LYS	2.7
1	I	507	GLU	2.7
1	H	126	GLY	2.7
1	L	347	GLY	2.7
1	D	194	SER	2.7
1	F	548	SER	2.7
1	J	588	PRO	2.7
1	K	580	SER	2.7
1	L	463	ARG	2.7
1	B	445	ILE	2.7
1	H	355	ILE	2.7
1	H	530	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	I	327	ILE	2.7
1	I	513	ILE	2.7
1	B	535	ALA	2.7
1	E	405	ALA	2.7
1	E	459	ASP	2.7
1	J	202	ASP	2.7
1	K	585	ALA	2.7
1	L	202	ASP	2.7
1	A	431	GLU	2.7
1	C	240	GLU	2.7
1	D	143	LYS	2.7
1	H	244	TYR	2.7
1	H	587	LYS	2.7
1	L	350	TYR	2.7
1	A	174	HIS	2.7
1	A	175	PHE	2.7
1	B	357	LEU	2.7
1	C	123	VAL	2.7
1	E	97	THR	2.7
1	E	224	VAL	2.7
1	F	128	THR	2.7
1	G	185	VAL	2.7
1	J	333	LEU	2.7
1	K	156	PHE	2.7
1	K	478	VAL	2.7
1	L	596	LEU	2.7
1	F	382	GLY	2.7
1	I	136	GLY	2.7
1	I	592	GLY	2.7
1	J	414	GLY	2.7
1	E	305	CYS	2.6
1	F	305	CYS	2.6
1	H	285	ARG	2.6
1	E	301	PRO	2.6
1	G	172	SER	2.6
1	J	100	PRO	2.6
1	L	309	SER	2.6
1	A	249	ASP	2.6
1	A	399	ASP	2.6
1	A	483	ASP	2.6
1	B	275	ASP	2.6
1	B	483	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	158	LYS	2.6
1	C	312	ASN	2.6
1	D	334	GLU	2.6
1	E	282	GLU	2.6
1	G	218	LYS	2.6
1	H	221	LYS	2.6
1	J	538	ASN	2.6
1	K	265	LYS	2.6
1	L	111	LYS	2.6
1	H	558	ALA	2.6
1	I	535	ALA	2.6
1	J	404	ALA	2.6
1	A	527	LEU	2.6
1	A	595	LEU	2.6
1	C	187	VAL	2.6
1	C	259	VAL	2.6
1	C	487	LEU	2.6
1	D	421	VAL	2.6
1	F	599	PHE	2.6
1	G	304	TYR	2.6
1	G	148	VAL	2.6
1	G	373	GLY	2.6
1	I	504	GLY	2.6
1	I	599	PHE	2.6
1	J	293	TYR	2.6
1	K	357	LEU	2.6
1	L	514	LEU	2.6
1	L	562	LEU	2.6
1	K	491	MET	2.6
1	L	213	MET	2.6
1	B	86	SER	2.6
1	B	401	SER	2.6
1	G	438	SER	2.6
1	K	539	SER	2.6
1	F	278	LYS	2.6
1	F	512	LYS	2.6
1	I	151	LYS	2.6
1	I	394	ASP	2.6
1	K	589	LYS	2.6
1	L	151	LYS	2.6
1	L	301	PRO	2.6
1	K	134	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	L	525	TRP	2.6
1	H	319	GLN	2.6
1	D	110	ILE	2.6
1	K	284	ALA	2.6
1	L	572	ALA	2.6
1	G	191	GLY	2.6
1	G	578	GLY	2.6
1	A	157	LEU	2.6
1	A	461	GLU	2.6
1	D	250	GLU	2.6
1	E	532	GLU	2.6
1	G	163	GLU	2.6
1	G	316	GLU	2.6
1	I	488	THR	2.6
1	A	478	VAL	2.6
1	B	478	VAL	2.6
1	D	167	VAL	2.6
1	F	94	LEU	2.6
1	F	210	LEU	2.6
1	G	472	TYR	2.6
1	H	287	TYR	2.6
1	I	346	LYS	2.6
1	L	103	TYR	2.6
1	L	245	GLU	2.6
1	J	91	VAL	2.6
1	B	494	SER	2.6
1	D	172	SER	2.6
1	J	146	SER	2.6
1	J	162	MET	2.6
1	B	307	PRO	2.6
1	E	152	GLN	2.6
1	F	568	ASN	2.6
1	G	149	ASN	2.6
1	H	384	ASN	2.6
1	I	296	GLN	2.6
1	A	440	ARG	2.6
1	C	500	ALA	2.6
1	D	577	ALA	2.6
1	I	251	ARG	2.6
1	C	126	GLY	2.6
1	F	140	GLY	2.6
1	G	216	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	343	SER	2.6
1	B	208	LEU	2.6
1	D	153	VAL	2.6
1	E	225	VAL	2.6
1	E	583	PHE	2.6
1	H	348	SER	2.6
1	H	559	SER	2.6
1	J	487	LEU	2.6
1	K	246	TYR	2.6
1	L	401	SER	2.6
1	B	338	MET	2.6
1	C	213	MET	2.6
1	F	400	MET	2.6
1	A	508	GLU	2.6
1	F	463	ARG	2.6
1	G	240	GLU	2.6
1	I	279	GLU	2.6
1	G	232	LYS	2.6
1	H	360	LYS	2.6
1	G	284	ALA	2.6
1	G	424	HIS	2.6
1	J	346	LYS	2.6
1	B	529	ILE	2.6
1	F	355	ILE	2.6
1	E	456	GLY	2.6
1	C	468	ASP	2.6
1	D	479	ASP	2.6
1	E	575	ASP	2.6
1	H	109	ASP	2.6
1	H	394	ASP	2.6
1	I	192	CYS	2.6
1	K	180	ASP	2.6
1	C	458	THR	2.6
1	G	105	THR	2.6
1	F	554	SER	2.6
1	I	273	ASN	2.6
1	K	520	SER	2.6
1	A	336	LEU	2.6
1	B	354	PHE	2.6
1	D	235	PHE	2.6
1	F	310	LEU	2.6
1	F	336	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	106	PRO	2.6
1	J	155	GLU	2.6
1	J	177	MET	2.6
1	J	330	VAL	2.6
1	L	175	PHE	2.6
1	A	189	TYR	2.6
1	B	111	LYS	2.6
1	C	204	LYS	2.6
1	C	512	LYS	2.6
1	D	440	ARG	2.6
1	I	240	GLU	2.6
1	E	436	LYS	2.6
1	F	584	LYS	2.6
1	C	570	ALA	2.6
1	E	340	ALA	2.6
1	I	170	GLY	2.6
1	K	318	ALA	2.6
1	F	468	ASP	2.6
1	F	546	GLN	2.6
1	D	128	THR	2.6
1	D	306	ASN	2.6
1	E	555	SER	2.6
1	K	97	THR	2.6
1	I	124	GLU	2.6
1	K	438	SER	2.6
1	B	317	LEU	2.6
1	F	509	LEU	2.6
1	H	323	LEU	2.6
1	I	464	LEU	2.6
1	I	523	PRO	2.6
1	K	528	PRO	2.6
1	L	441	PRO	2.6
1	A	349	MET	2.6
1	A	491	MET	2.6
1	F	433	MET	2.6
1	G	503	PHE	2.6
1	L	226	PHE	2.6
1	D	383	TYR	2.6
1	E	387	ALA	2.6
1	F	313	ALA	2.6
1	F	496	GLY	2.6
1	I	284	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	163	GLU	2.6
1	B	547	ILE	2.6
1	H	582	ASN	2.6
1	I	218	LYS	2.6
1	I	436	LYS	2.6
1	K	173	LYS	2.6
1	A	209	SER	2.5
1	D	212	THR	2.5
1	G	534	ARG	2.5
1	I	415	THR	2.5
1	J	309	SER	2.5
1	J	497	THR	2.5
1	A	413	VAL	2.5
1	D	213	MET	2.5
1	F	91	VAL	2.5
1	F	213	MET	2.5
1	G	482	VAL	2.5
1	H	92	VAL	2.5
1	H	344	VAL	2.5
1	J	561	PHE	2.5
1	C	249	ASP	2.5
1	G	364	ASP	2.5
1	H	515	GLN	2.5
1	I	215	HIS	2.5
1	A	347	GLY	2.5
1	C	461	GLU	2.5
1	H	240	GLU	2.5
1	H	442	GLY	2.5
1	J	345	GLY	2.5
1	J	496	GLY	2.5
1	K	125	GLU	2.5
1	L	143	LYS	2.5
1	A	457	ASN	2.5
1	F	294	ALA	2.5
1	H	303	ASN	2.5
1	H	404	ALA	2.5
1	I	122	ASN	2.5
1	K	473	ALA	2.5
1	A	251	ARG	2.5
1	A	534	ARG	2.5
1	B	236	ARG	2.5
1	E	154	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	438	SER	2.5
1	J	93	SER	2.5
1	H	528	PRO	2.5
1	E	131	LEU	2.5
1	F	208	LEU	2.5
1	F	250	GLU	2.5
1	F	514	LEU	2.5
1	G	371	LEU	2.5
1	G	476	LEU	2.5
1	I	543	ASP	2.5
1	K	321	LEU	2.5
1	L	543	ASP	2.5
1	A	177	MET	2.5
1	B	593	VAL	2.5
1	C	235	PHE	2.5
1	C	339	GLY	2.5
1	D	126	GLY	2.5
1	D	140	GLY	2.5
1	G	566	VAL	2.5
1	H	170	GLY	2.5
1	H	504	GLY	2.5
1	I	315	VAL	2.5
1	J	140	GLY	2.5
1	K	281	VAL	2.5
1	D	403	CYS	2.5
1	D	260	ASN	2.5
1	F	303	ASN	2.5
1	K	181	ASN	2.5
1	K	277	TYR	2.5
1	K	594	ARG	2.5
1	L	411	TYR	2.5
1	L	521	ASN	2.5
1	I	447	ALA	2.5
1	A	199	SER	2.5
1	B	172	SER	2.5
1	E	199	SER	2.5
1	J	516	SER	2.5
1	A	223	THR	2.5
1	H	248	THR	2.5
1	I	556	ILE	2.5
1	D	567	GLN	2.5
1	E	113	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	100	PRO	2.5
1	J	522	GLU	2.5
1	B	204	LYS	2.5
1	C	164	LYS	2.5
1	C	216	ASP	2.5
1	K	374	LYS	2.5
1	L	218	LYS	2.5
1	C	208	LEU	2.5
1	I	267	LEU	2.5
1	L	266	HIS	2.5
1	D	568	ASN	2.5
1	E	179	ASN	2.5
1	G	349	MET	2.5
1	I	425	PHE	2.5
1	J	142	VAL	2.5
1	J	179	ASN	2.5
1	K	354	PHE	2.5
1	L	104	ASN	2.5
1	L	203	MET	2.5
1	A	340	ALA	2.5
1	D	500	ALA	2.5
1	E	439	TYR	2.5
1	F	194	SER	2.5
1	F	288	TYR	2.5
1	C	282	GLU	2.5
1	C	454	GLU	2.5
1	C	474	GLU	2.5
1	F	448	SER	2.5
1	G	517	SER	2.5
1	J	201	ALA	2.5
1	H	160	GLU	2.5
1	L	86	SER	2.5
1	B	296	GLN	2.5
1	B	319	GLN	2.5
1	H	164	LYS	2.5
1	J	296	GLN	2.5
1	C	519	THR	2.5
1	F	483	ASP	2.5
1	H	488	THR	2.5
1	L	446	THR	2.5
1	G	100	PRO	2.5
1	L	440	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	306	ASN	2.5
1	D	437	ASN	2.5
1	D	538	ASN	2.5
1	E	408	GLY	2.5
1	I	306	ASN	2.5
1	I	342	LEU	2.5
1	B	125	GLU	2.5
1	D	503	PHE	2.5
1	E	461	GLU	2.5
1	F	247	MET	2.5
1	F	422	GLU	2.5
1	H	566	VAL	2.5
1	B	587	LYS	2.5
1	E	563	LYS	2.5
1	D	300	ALA	2.5
1	D	361	SER	2.5
1	D	374	LYS	2.5
1	B	500	ALA	2.5
1	D	572	ALA	2.5
1	E	86	SER	2.5
1	I	314	ALA	2.5
1	K	370	ALA	2.5
1	K	494	SER	2.5
1	B	244	TYR	2.5
1	E	189	TYR	2.5
1	I	216	ASP	2.5
1	D	446	THR	2.5
1	J	569	THR	2.5
1	K	463	ARG	2.5
1	B	544	ILE	2.5
1	E	423	ILE	2.5
1	B	126	GLY	2.5
1	J	375	GLY	2.5
1	D	240	GLU	2.5
1	C	198	LEU	2.5
1	D	218	LYS	2.5
1	K	169	LEU	2.5
1	D	400	MET	2.5
1	E	338	MET	2.5
1	G	515	GLN	2.5
1	A	302	SER	2.5
1	C	391	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	220	SER	2.5
1	G	494	SER	2.5
1	K	112	VAL	2.5
1	K	285	ARG	2.5
1	F	103	TYR	2.5
1	G	418	PRO	2.5
1	I	141	PRO	2.5
1	J	241	THR	2.5
1	C	511	ASN	2.5
1	D	522	GLU	2.5
1	E	280	GLU	2.5
1	J	545	ASN	2.5
1	J	151	LYS	2.5
1	J	290	GLY	2.5
1	J	386	LYS	2.5
1	L	110	ILE	2.5
1	L	204	LYS	2.5
1	L	436	LYS	2.5
1	B	567	GLN	2.5
1	E	90	GLN	2.5
1	A	476	LEU	2.5
1	A	575	ASP	2.5
1	G	527	LEU	2.5
1	H	342	LEU	2.5
1	E	184	SER	2.4
1	F	520	SER	2.4
1	H	380	SER	2.4
1	I	86	SER	2.4
1	L	209	SER	2.4
1	A	114	VAL	2.4
1	C	463	ARG	2.4
1	D	251	ARG	2.4
1	C	156	PHE	2.4
1	B	163	GLU	2.4
1	C	572	ALA	2.4
1	H	370	ALA	2.4
1	I	467	ALA	2.4
1	I	585	ALA	2.4
1	J	434	VAL	2.4
1	K	132	VAL	2.4
1	L	227	GLU	2.4
1	L	598	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	441	PRO	2.4
1	D	253	LYS	2.4
1	F	521	ASN	2.4
1	I	278	LYS	2.4
1	I	432	ASN	2.4
1	I	446	THR	2.4
1	I	449	ASN	2.4
1	J	307	PRO	2.4
1	K	418	PRO	2.4
1	K	526	TRP	2.4
1	B	573	HIS	2.4
1	C	472	TYR	2.4
1	L	288	TYR	2.4
1	F	544	ILE	2.4
1	G	369	ILE	2.4
1	I	319	GLN	2.4
1	I	546	GLN	2.4
1	K	159	ASP	2.4
1	A	93	SER	2.4
1	D	586	ARG	2.4
1	C	357	LEU	2.4
1	E	125	GLU	2.4
1	G	86	SER	2.4
1	I	586	ARG	2.4
1	J	371	LEU	2.4
1	K	532	GLU	2.4
1	C	182	LYS	2.4
1	C	552	LYS	2.4
1	K	162	MET	2.4
1	A	421	VAL	2.4
1	D	482	VAL	2.4
1	G	490	ALA	2.4
1	J	500	ALA	2.4
1	K	553	ALA	2.4
1	L	308	VAL	2.4
1	C	456	GLY	2.4
1	I	191	GLY	2.4
1	I	489	GLY	2.4
1	J	536	THR	2.4
1	D	459	ASP	2.4
1	F	379	ASP	2.4
1	L	249	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	564	GLU	2.4
1	C	102	GLU	2.4
1	C	245	GLU	2.4
1	F	236	ARG	2.4
1	I	481	ILE	2.4
1	D	204	LYS	2.4
1	D	540	LYS	2.4
1	K	380	SER	2.4
1	K	397	LYS	2.4
1	D	328	LEU	2.4
1	G	305	CYS	2.4
1	I	104	ASN	2.4
1	K	183	ASN	2.4
1	L	602	ASN	2.4
1	E	553	ALA	2.4
1	G	319	GLN	2.4
1	J	313	ALA	2.4
1	J	447	ALA	2.4
1	K	201	ALA	2.4
1	A	132	VAL	2.4
1	A	237	PHE	2.4
1	A	482	VAL	2.4
1	A	502	VAL	2.4
1	B	408	GLY	2.4
1	D	96	PRO	2.4
1	H	579	VAL	2.4
1	H	592	GLY	2.4
1	I	266	HIS	2.4
1	J	225	VAL	2.4
1	K	225	VAL	2.4
1	E	590	GLY	2.4
1	I	248	THR	2.4
1	L	290	GLY	2.4
1	G	251	ARG	2.4
1	A	368	LYS	2.4
1	C	360	LYS	2.4
1	C	499	TYR	2.4
1	K	288	TYR	2.4
1	I	199	SER	2.4
1	J	311	SER	2.4
1	A	514	LEU	2.4
1	A	596	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	210	LEU	2.4
1	C	272	ASN	2.4
1	I	395	LEU	2.4
1	I	476	LEU	2.4
1	F	431	GLU	2.4
1	H	490	ALA	2.4
1	K	507	GLU	2.4
1	A	301	PRO	2.4
1	B	455	VAL	2.4
1	D	158	LYS	2.4
1	D	569	THR	2.4
1	E	173	LYS	2.4
1	F	565	PHE	2.4
1	H	459	ASP	2.4
1	J	212	THR	2.4
1	K	130	PHE	2.4
1	K	197	ASP	2.4
1	G	366	LYS	2.4
1	H	552	LYS	2.4
1	I	552	LYS	2.4
1	C	380	SER	2.4
1	D	427	SER	2.4
1	A	510	ILE	2.4
1	D	481	ILE	2.4
1	A	303	ASN	2.4
1	C	303	ASN	2.4
1	D	525	TRP	2.4
1	H	350	TYR	2.4
1	E	322	ASN	2.4
1	E	531	ASN	2.4
1	K	449	ASN	2.4
1	I	324	GLU	2.4
1	C	267	LEU	2.4
1	C	470	LEU	2.4
1	J	357	LEU	2.4
1	K	242	LEU	2.4
1	L	595	LEU	2.4
1	C	108	HIS	2.4
1	C	390	GLY	2.4
1	E	552	LYS	2.4
1	G	326	LYS	2.4
1	J	158	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	K	158	LYS	2.4
1	E	314	ALA	2.4
1	G	400	MET	2.4
1	J	433	MET	2.4
1	L	573	HIS	2.4
1	B	536	THR	2.4
1	C	175	PHE	2.4
1	D	112	VAL	2.4
1	D	165	PHE	2.4
1	D	276	THR	2.4
1	B	454	GLU	2.4
1	D	282	GLU	2.4
1	E	435	SER	2.4
1	J	507	GLU	2.4
1	E	350	TYR	2.4
1	E	444	ILE	2.4
1	E	530	ILE	2.4
1	F	445	ILE	2.4
1	G	383	TYR	2.4
1	G	513	ILE	2.4
1	K	360	LYS	2.4
1	A	216	ASP	2.4
1	H	251	ARG	2.4
1	J	285	ARG	2.4
1	K	586	ARG	2.4
1	E	578	GLY	2.4
1	L	339	GLY	2.4
1	K	222	LEU	2.4
1	H	300	ALA	2.4
1	B	488	THR	2.4
1	J	223	THR	2.4
1	L	569	THR	2.4
1	B	124	GLU	2.4
1	D	156	PHE	2.4
1	H	454	GLU	2.4
1	I	282	GLU	2.4
1	I	461	GLU	2.4
1	L	524	VAL	2.4
1	A	512	LYS	2.3
1	C	154	SER	2.4
1	E	582	ASN	2.4
1	F	218	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	437	ASN	2.4
1	K	366	LYS	2.3
1	L	302	SER	2.4
1	E	197	ASP	2.3
1	E	271	ILE	2.3
1	E	533	TYR	2.3
1	J	288	TYR	2.3
1	J	402	GLY	2.3
1	A	328	LEU	2.3
1	F	262	GLU	2.3
1	G	89	PRO	2.3
1	G	500	ALA	2.3
1	J	461	GLU	2.3
1	K	200	GLU	2.3
1	L	469	ALA	2.3
1	L	588	PRO	2.3
1	C	152	GLN	2.3
1	I	338	MET	2.3
1	D	346	LYS	2.3
1	K	475	LYS	2.3
1	L	353	LYS	2.3
1	B	502	VAL	2.3
1	E	254	SER	2.3
1	H	516	SER	2.3
1	I	427	SER	2.3
1	J	438	SER	2.3
1	K	330	VAL	2.3
1	B	414	GLY	2.3
1	A	419	GLU	2.3
1	H	453	ILE	2.3
1	I	125	GLU	2.3
1	A	320	LYS	2.3
1	D	89	PRO	2.3
1	I	221	LYS	2.3
1	I	389	PRO	2.3
1	J	246	TYR	2.3
1	K	480	TYR	2.3
1	C	371	LEU	2.3
1	L	232	LYS	2.3
1	A	358	THR	2.3
1	E	233	ASN	2.3
1	E	516	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	199	SER	2.3
1	F	580	SER	2.3
1	B	206	VAL	2.3
1	D	206	VAL	2.3
1	D	394	ASP	2.3
1	E	142	VAL	2.3
1	F	425	PHE	2.3
1	K	92	VAL	2.3
1	A	170	GLY	2.3
1	B	456	GLY	2.3
1	H	382	GLY	2.3
1	K	347	GLY	2.3
1	A	337	LYS	2.3
1	I	518	LYS	2.3
1	J	366	LYS	2.3
1	K	436	LYS	2.3
1	C	327	ILE	2.3
1	E	264	ILE	2.3
1	G	529	ILE	2.3
1	E	389	PRO	2.3
1	A	217	ASN	2.3
1	A	333	LEU	2.3
1	A	463	ARG	2.3
1	A	506	ASN	2.3
1	B	359	TYR	2.3
1	C	384	ASN	2.3
1	E	469	ALA	2.3
1	I	457	ASN	2.3
1	J	472	TYR	2.3
1	C	452	THR	2.3
1	E	465	THR	2.3
1	G	212	THR	2.3
1	G	536	THR	2.3
1	J	446	THR	2.3
1	G	245	GLU	2.3
1	K	316	GLU	2.3
1	B	442	GLY	2.3
1	B	561	PHE	2.3
1	C	113	GLN	2.3
1	C	120	GLY	2.3
1	D	329	GLY	2.3
1	E	353	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	397	LYS	2.3
1	G	346	LYS	2.3
1	G	502	VAL	2.3
1	H	413	VAL	2.3
1	I	462	GLY	2.3
1	K	215	HIS	2.3
1	D	100	PRO	2.3
1	I	351	PRO	2.3
1	K	523	PRO	2.3
1	J	139	ASN	2.3
1	D	543	ASP	2.3
1	E	249	ASP	2.3
1	H	535	ALA	2.3
1	D	127	LEU	2.3
1	F	212	THR	2.3
1	F	292	TYR	2.3
1	J	480	TYR	2.3
1	K	435	SER	2.3
1	C	353	LYS	2.3
1	D	247	MET	2.3
1	F	397	LYS	2.3
1	I	203	MET	2.3
1	K	563	LYS	2.3
1	C	373	GLY	2.3
1	F	489	GLY	2.3
1	G	477	GLY	2.3
1	J	152	GLN	2.3
1	K	345	GLY	2.3
1	D	266	HIS	2.3
1	D	413	VAL	2.3
1	I	156	PHE	2.3
1	L	108	HIS	2.3
1	J	594	ARG	2.3
1	D	303	ASN	2.3
1	G	454	GLU	2.3
1	D	249	ASP	2.3
1	G	96	PRO	2.3
1	I	538	ASN	2.3
1	E	164	LYS	2.3
1	E	331	LYS	2.3
1	B	577	ALA	2.3
1	D	314	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	348	SER	2.3
1	E	93	SER	2.3
1	E	333	LEU	2.3
1	F	248	THR	2.3
1	F	427	SER	2.3
1	G	302	SER	2.3
1	I	555	SER	2.3
1	J	295	SER	2.3
1	L	542	ALA	2.3
1	L	171	THR	2.3
1	I	189	TYR	2.3
1	C	329	GLY	2.3
1	G	489	GLY	2.3
1	H	339	GLY	2.3
1	J	373	GLY	2.3
1	K	193	GLY	2.3
1	H	108	HIS	2.3
1	H	356	HIS	2.3
1	F	406	VAL	2.3
1	I	455	VAL	2.3
1	C	538	ASN	2.3
1	A	326	LYS	2.3
1	D	265	LYS	2.3
1	D	254	SER	2.3
1	D	460	ALA	2.3
1	D	498	SER	2.3
1	K	343	SER	2.3
1	L	186	ALA	2.3
1	F	358	THR	2.2
1	A	240	GLU	2.2
1	C	251	ARG	2.2
1	C	268	GLY	2.2
1	C	347	GLY	2.2
1	D	193	GLY	2.2
1	E	126	GLY	2.2
1	E	193	GLY	2.2
1	E	236	ARG	2.2
1	H	373	GLY	2.2
1	J	332	GLU	2.2
1	L	163	GLU	2.2
1	G	433	MET	2.2
1	C	409	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	412	CYS	2.2
1	E	337	LYS	2.2
1	H	589	LYS	2.2
1	K	109	ASP	2.2
1	K	575	ASP	2.2
1	A	566	VAL	2.2
1	E	269	VAL	2.2
1	J	482	VAL	2.2
1	D	307	PRO	2.2
1	F	523	PRO	2.2
1	H	418	PRO	2.2
1	C	319	GLN	2.2
1	C	87	GLU	2.2
1	E	380	SER	2.2
1	H	494	SER	2.2
1	G	228	ILE	2.2
1	H	532	GLU	2.2
1	J	200	GLU	2.2
1	D	469	ALA	2.2
1	J	264	ILE	2.2
1	J	191	GLY	2.2
1	L	223	THR	2.2
1	D	416	LEU	2.2
1	D	589	LYS	2.2
1	E	168	LYS	2.2
1	E	336	LEU	2.2
1	G	509	LEU	2.2
1	E	176	TYR	2.2
1	G	189	TYR	2.2
1	G	203	MET	2.2
1	H	449	ASN	2.2
1	L	399	ASP	2.2
1	L	457	ASN	2.2
1	D	237	PHE	2.2
1	E	141	PRO	2.2
1	E	503	PHE	2.2
1	C	172	SER	2.2
1	G	265	LYS	2.2
1	H	397	LYS	2.2
1	I	353	LYS	2.2
1	L	386	LYS	2.2
1	A	105	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	423	ILE	2.2
1	D	513	ILE	2.2
1	I	373	GLY	2.2
1	L	381	GLY	2.2
1	L	415	THR	2.2
1	E	159	ASP	2.2
1	F	166	ASN	2.2
1	G	352	ASN	2.2
1	L	506	ASN	2.2
1	C	359	TYR	2.2
1	C	532	GLU	2.2
1	K	124	GLU	2.2
1	K	287	TYR	2.2
1	H	389	PRO	2.2
1	A	88	VAL	2.2
1	E	366	LYS	2.2
1	F	386	LYS	2.2
1	A	498	SER	2.2
1	E	348	SER	2.2
1	I	517	SER	2.2
1	K	498	SER	2.2
1	A	381	GLY	2.2
1	I	126	GLY	2.2
1	I	442	GLY	2.2
1	L	450	GLY	2.2
1	A	521	ASN	2.2
1	A	597	THR	2.2
1	B	453	ILE	2.2
1	F	171	THR	2.2
1	L	314	ALA	2.2
1	F	217	ASN	2.2
1	E	316	GLU	2.2
1	J	215	HIS	2.2
1	B	169	LEU	2.2
1	H	296	GLN	2.2
1	E	147	LYS	2.2
1	H	586	ARG	2.2
1	K	151	LYS	2.2
1	H	325	TYR	2.2
1	C	254	SER	2.2
1	C	539	SER	2.2
1	E	88	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	438	SER	2.2
1	L	482	VAL	2.2
1	H	381	GLY	2.2
1	C	569	THR	2.2
1	D	174	HIS	2.2
1	D	424	HIS	2.2
1	D	458	THR	2.2
1	H	572	ALA	2.2
1	J	356	HIS	2.2
1	J	490	ALA	2.2
1	L	291	THR	2.2
1	F	556	ILE	2.2
1	A	278	LYS	2.2
1	D	169	LEU	2.2
1	D	534	ARG	2.2
1	I	236	ARG	2.2
1	J	374	LYS	2.2
1	F	239	LEU	2.2
1	J	317	LEU	2.2
1	J	336	LEU	2.2
1	F	588	PRO	2.2
1	J	141	PRO	2.2
1	K	135	PRO	2.2
1	C	548	SER	2.2
1	D	199	SER	2.2
1	D	559	SER	2.2
1	G	209	SER	2.2
1	G	262	GLU	2.2
1	K	245	GLU	2.2
1	L	517	SER	2.2
1	D	382	GLY	2.2
1	D	582	ASN	2.2
1	J	133	ASN	2.2
1	J	281	VAL	2.2
1	K	566	VAL	2.2
1	F	354	PHE	2.2
1	J	583	PHE	2.2
1	B	589	LYS	2.2
1	A	291	THR	2.2
1	C	284	ALA	2.2
1	C	469	ALA	2.2
1	H	368	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	K	536	THR	2.2
1	K	573	HIS	2.2
1	L	326	LYS	2.2
1	F	440	ARG	2.2
1	D	327	ILE	2.2
1	K	267	LEU	2.2
1	E	247	MET	2.2
1	J	247	MET	2.2
1	I	548	SER	2.2
1	J	520	SER	2.2
1	L	438	SER	2.2
1	F	450	GLY	2.2
1	I	181	ASN	2.1
1	J	134	ASN	2.1
1	L	346	LYS	2.1
1	B	288	TYR	2.1
1	F	246	TYR	2.1
1	J	287	TYR	2.1
1	D	344	VAL	2.1
1	G	206	VAL	2.1
1	J	425	PHE	2.1
1	K	358	THR	2.1
1	C	227	GLU	2.1
1	E	522	GLU	2.1
1	J	445	ILE	2.1
1	C	321	LEU	2.1
1	J	169	LEU	2.1
1	J	249	ASP	2.1
1	A	204	LYS	2.1
1	B	563	LYS	2.1
1	D	517	SER	2.1
1	F	343	SER	2.1
1	G	147	LYS	2.1
1	H	168	LYS	2.1
1	J	351	PRO	2.1
1	A	568	ASN	2.1
1	C	592	GLY	2.1
1	E	568	ASN	2.1
1	F	290	GLY	2.1
1	F	329	GLY	2.1
1	I	188	GLY	2.1
1	I	545	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	J	602	ASN	2.1
1	K	177	MET	2.1
1	K	303	ASN	2.1
1	L	352	ASN	2.1
1	A	282	GLU	2.1
1	B	341	TYR	2.1
1	G	356	HIS	2.1
1	G	471	VAL	2.1
1	H	502	VAL	2.1
1	I	334	GLU	2.1
1	L	246	TYR	2.1
1	C	91	VAL	2.1
1	D	330	VAL	2.1
1	F	206	VAL	2.1
1	C	186	ALA	2.1
1	G	235	PHE	2.1
1	H	388	ALA	2.1
1	E	221	LYS	2.1
1	I	483	ASP	2.1
1	J	111	LYS	2.1
1	J	118	LYS	2.1
1	L	320	LYS	2.1
1	J	129	ILE	2.1
1	D	242	LEU	2.1
1	E	122	ASN	2.1
1	E	134	ASN	2.1
1	H	183	ASN	2.1
1	I	172	SER	2.1
1	E	347	GLY	2.1
1	G	126	GLY	2.1
1	J	504	GLY	2.1
1	L	303	ASN	2.1
1	L	338	MET	2.1
1	C	334	GLU	2.1
1	E	508	GLU	2.1
1	H	334	GLU	2.1
1	I	245	GLU	2.1
1	A	92	VAL	2.1
1	A	265	LYS	2.1
1	B	325	TYR	2.1
1	B	460	ALA	2.1
1	D	241	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	269	VAL	2.1
1	D	478	VAL	2.1
1	F	147	LYS	2.1
1	G	340	ALA	2.1
1	H	367	LYS	2.1
1	H	458	THR	2.1
1	J	253	LYS	2.1
1	D	515	GLN	2.1
1	E	156	PHE	2.1
1	L	238	PHE	2.1
1	L	483	ASP	2.1
1	B	139	ASN	2.1
1	E	494	SER	2.1
1	H	327	ILE	2.1
1	J	539	SER	2.1
1	J	568	ASN	2.1
1	K	437	ASN	2.1
1	K	506	ASN	2.1
1	L	389	PRO	2.1
1	H	349	MET	2.1
1	K	108	HIS	2.1
1	C	525	TRP	2.1
1	C	459	ASP	2.1
1	A	585	ALA	2.1
1	C	224	VAL	2.1
1	C	340	ALA	2.1
1	C	490	ALA	2.1
1	E	458	THR	2.1
1	C	205	ARG	2.1
1	F	383	TYR	2.1
1	C	243	PHE	2.1
1	D	425	PHE	2.1
1	F	324	GLU	2.1
1	J	102	GLU	2.1
1	J	586	ARG	2.1
1	K	568	ASN	2.1
1	A	539	SER	2.1
1	D	501	GLY	2.1
1	F	172	SER	2.1
1	F	456	GLY	2.1
1	G	311	SER	2.1
1	H	220	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	L	489	GLY	2.1
1	F	327	ILE	2.1
1	H	529	ILE	2.1
1	B	540	LYS	2.1
1	I	118	LYS	2.1
1	J	182	LYS	2.1
1	I	174	HIS	2.1
1	D	399	ASP	2.1
1	C	212	THR	2.1
1	C	534	ARG	2.1
1	D	431	GLU	2.1
1	E	519	THR	2.1
1	H	97	THR	2.1
1	G	322	ASN	2.1
1	J	166	ASN	2.1
1	E	211	VAL	2.1
1	K	471	VAL	2.1
1	B	290	GLY	2.1
1	B	309	SER	2.1
1	C	103	TYR	2.1
1	C	253	LYS	2.1
1	C	326	LYS	2.1
1	C	477	GLY	2.1
1	E	232	LYS	2.1
1	E	339	GLY	2.1
1	F	189	TYR	2.1
1	I	254	SER	2.1
1	J	176	TYR	2.1
1	J	302	SER	2.1
1	J	456	GLY	2.1
1	L	539	SER	2.1
1	B	546	GLN	2.1
1	J	210	LEU	2.1
1	K	94	LEU	2.1
1	A	262	GLU	2.1
1	B	332	GLU	2.1
1	D	216	ASP	2.1
1	I	468	ASP	2.1
1	I	479	ASP	2.1
1	K	479	ASP	2.1
1	L	454	GLU	2.1
1	K	251	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	183	ASN	2.1
1	D	415	THR	2.1
1	D	505	ASN	2.1
1	A	173	LYS	2.1
1	A	428	ALA	2.1
1	A	475	LYS	2.1
1	E	223	THR	2.1
1	I	312	ASN	2.1
1	K	272	ASN	2.1
1	C	535	ALA	2.1
1	E	201	ALA	2.1
1	K	164	LYS	2.1
1	L	563	LYS	2.1
1	A	153	VAL	2.1
1	B	170	GLY	2.1
1	C	478	VAL	2.1
1	D	375	GLY	2.1
1	G	414	GLY	2.1
1	H	578	GLY	2.1
1	K	194	SER	2.1
1	L	501	GLY	2.1
1	F	130	PHE	2.1
1	G	564	GLU	2.0
1	J	459	ASP	2.0
1	L	443	ASP	2.0
1	D	594	ARG	2.0
1	K	423	ILE	2.0
1	E	253	LYS	2.0
1	F	552	LYS	2.0
1	G	338	MET	2.0
1	H	204	LYS	2.0
1	H	213	MET	2.0
1	J	540	LYS	2.0
1	L	166	ASN	2.0
1	L	247	MET	2.0
1	F	473	ALA	2.0
1	H	345	GLY	2.0
1	I	428	ALA	2.0
1	A	380	SER	2.0
1	D	98	SER	2.0
1	F	517	SER	2.0
1	I	448	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	K	422	GLU	2.0
1	L	427	SER	2.0
1	A	142	VAL	2.0
1	B	92	VAL	2.0
1	D	141	PRO	2.0
1	L	412	CYS	2.0
1	D	436	LYS	2.0
1	J	589	LYS	2.0
1	C	453	ILE	2.0
1	K	234	LEU	2.0
1	J	506	ASN	2.0
1	A	261	MET	2.0
1	G	431	GLU	2.0
1	J	87	GLU	2.0
1	L	522	GLU	2.0
1	B	347	GLY	2.0
1	E	191	GLY	2.0
1	F	442	GLY	2.0
1	J	113	GLN	2.0
1	J	171	THR	2.0
1	D	295	SER	2.0
1	H	98	SER	2.0
1	J	570	ALA	2.0
1	A	89	PRO	2.0
1	A	418	PRO	2.0
1	E	479	ASP	2.0
1	J	479	ASP	2.0
1	B	326	LYS	2.0
1	C	561	PHE	2.0
1	D	238	PHE	2.0
1	C	545	ASN	2.0
1	E	246	TYR	2.0
1	J	322	ASN	2.0
1	C	332	GLU	2.0
1	D	117	ILE	2.0
1	G	474	GLU	2.0
1	L	334	GLU	2.0
1	L	357	LEU	2.0
1	B	402	GLY	2.0
1	I	119	GLY	2.0
1	I	414	GLY	2.0
1	K	477	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	563	LYS	2.0
1	E	205	ARG	2.0
1	H	236	ARG	2.0
1	J	199	SER	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
7	SO4	C	711	5/5	0.31	1.43	20.10	41,45,53,55	0
5	1PE	B	705	10/16	0.31	0.69	9.96	36,40,51,51	0
7	SO4	F	707	5/5	0.39	0.79	9.06	55,57,61,75	0
7	SO4	C	710	5/5	0.71	0.85	8.66	34,38,58,62	0
7	SO4	A	711	5/5	0.22	0.72	8.04	56,56,63,81	0
5	1PE	L	705	7/16	0.44	0.90	7.67	30,34,39,41	0
5	1PE	H	706	10/16	0.53	0.61	6.38	30,40,46,47	0
2	CO3	D	701	4/4	0.75	0.58	5.78	16,17,18,18	0
7	SO4	C	708	5/5	-0.01	0.66	4.67	53,57,64,72	0
7	SO4	E	709	5/5	0.50	0.46	4.44	47,51,64,76	0
7	SO4	A	712	5/5	0.73	0.66	3.99	36,42,50,54	0
2	CO3	E	701	4/4	0.83	0.48	3.76	16,18,18,21	0
5	1PE	K	706	12/16	0.47	0.39	3.22	26,36,43,48	0
7	SO4	G	711	5/5	0.53	0.60	3.09	46,48,51,55	0
5	1PE	D	706	10/16	0.58	0.46	3.08	27,36,40,41	0
2	CO3	K	701	4/4	0.68	0.47	3.06	19,19,19,21	0
7	SO4	K	708	5/5	0.22	0.51	2.79	58,60,74,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CO3	J	701	4/4	0.79	0.46	2.78	15,16,17,20	0
5	1PE	I	706	11/16	0.46	0.42	2.28	26,35,48,53	0
5	1PE	J	707	10/16	0.46	0.44	1.94	27,34,42,52	0
5	1PE	A	705	9/16	0.63	0.55	1.94	25,32,36,39	0
2	CO3	I	701	4/4	0.88	0.38	1.91	15,15,16,17	0
4	4ZN	D	704	20/20	0.54	0.43	1.76	13,20,27,31	3
5	1PE	G	705	9/16	0.49	0.52	1.75	25,32,39,40	0
4	4ZN	B	704	16/20	0.55	0.43	1.59	11,19,24,31	3
5	1PE	G	706	6/16	0.70	0.41	1.58	34,37,41,42	0
5	1PE	C	706	9/16	0.67	0.35	1.57	26,29,35,36	0
5	1PE	F	705	10/16	0.40	0.39	1.39	26,37,45,52	0
5	1PE	G	707	6/16	0.49	0.45	1.34	31,35,39,39	0
5	1PE	L	706	10/16	0.66	0.39	1.21	31,38,45,48	0
4	4ZN	G	704	16/20	0.53	0.44	0.98	14,17,22,23	4
5	1PE	J	705	11/16	0.25	0.42	0.96	33,40,50,52	0
4	4ZN	F	704	16/20	0.53	0.42	0.95	17,21,27,31	3
5	1PE	E	706	12/16	0.53	0.38	0.90	25,33,43,44	0
4	4ZN	L	704	16/20	0.53	0.44	0.86	14,18,23,27	3
4	4ZN	E	704	20/20	0.69	0.42	0.84	16,20,27,28	7
4	4ZN	H	704	16/20	0.70	0.42	0.83	12,18,28,32	3
4	4ZN	C	704	16/20	0.69	0.38	0.73	15,18,23,24	4
4	4ZN	K	704	14/20	0.56	0.39	0.50	14,20,28,33	0
2	CO3	C	701	4/4	0.54	0.37	0.46	15,16,18,18	0
7	SO4	E	707	5/5	0.91	0.37	0.40	21,21,23,24	0
4	4ZN	I	704	12/20	0.69	0.34	0.29	16,18,22,23	0
2	CO3	B	701	4/4	0.74	0.33	0.23	16,16,16,20	0
7	SO4	A	708	5/5	0.60	0.43	0.21	44,47,50,58	0
2	CO3	L	701	4/4	0.60	0.37	0.12	16,17,18,19	0
7	SO4	G	709	5/5	0.92	0.33	0.03	16,19,20,22	0
7	SO4	J	708	5/5	0.95	0.31	-0.04	21,22,24,25	0
4	4ZN	A	704	16/20	0.60	0.37	-0.10	15,17,22,23	3
2	CO3	H	701	4/4	0.67	0.34	-0.17	15,16,17,19	0
7	SO4	A	709	5/5	0.73	0.35	-0.23	53,57,75,78	0
7	SO4	I	708	5/5	0.68	0.30	-0.35	74,74,83,91	0
4	4ZN	J	704	16/20	0.73	0.29	-0.49	14,17,21,27	3
7	SO4	A	710	5/5	0.73	0.33	-0.54	36,40,54,59	0
2	CO3	G	701	4/4	0.62	0.33	-0.63	13,14,17,19	0
2	CO3	F	701	4/4	0.56	0.30	-0.76	19,19,19,20	0
7	SO4	B	707	5/5	0.93	0.25	-1.11	17,19,23,24	0
2	CO3	A	701	4/4	0.72	0.29	-1.58	15,18,19,20	0
3	ZN	L	702	1/1	0.61	0.22	-1.67	18,18,18,18	0
7	SO4	G	710	5/5	0.75	0.21	-2.18	35,43,55,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	ZN	I	702	1/1	0.22	0.14	-2.52	19,19,19,19	0
3	ZN	C	702	1/1	0.53	0.17	-2.76	19,19,19,19	0
3	ZN	B	703	1/1	0.90	0.08	-3.18	15,15,15,15	0
3	ZN	K	703	1/1	0.92	0.14	-3.26	16,16,16,16	0
3	ZN	C	703	1/1	0.74	0.12	-3.27	15,15,15,15	0
3	ZN	L	703	1/1	0.88	0.11	-3.30	17,17,17,17	0
3	ZN	H	703	1/1	0.69	0.10	-3.33	15,15,15,15	0
3	ZN	F	702	1/1	0.58	0.14	-3.48	22,22,22,22	0
3	ZN	K	702	1/1	0.91	0.09	-3.57	19,19,19,19	0
3	ZN	J	703	1/1	0.72	0.10	-3.68	15,15,15,15	0
3	ZN	H	702	1/1	0.73	0.08	-3.85	17,17,17,17	0
3	ZN	B	702	1/1	0.87	0.06	-3.86	17,17,17,17	0
3	ZN	D	703	1/1	0.82	0.10	-4.04	17,17,17,17	0
3	ZN	I	703	1/1	0.60	0.07	-4.19	19,19,19,19	0
3	ZN	E	702	1/1	0.95	0.07	-4.82	17,17,17,17	0
3	ZN	G	702	1/1	0.69	0.10	-4.85	18,18,18,18	0
3	ZN	G	703	1/1	0.82	0.09	-4.85	15,15,15,15	0
3	ZN	J	702	1/1	0.71	0.09	-4.89	19,19,19,19	0
3	ZN	F	703	1/1	0.97	0.08	-5.07	18,18,18,18	0
3	ZN	A	703	1/1	0.82	0.10	-5.13	14,14,14,14	0
3	ZN	A	702	1/1	0.67	0.16	-5.24	18,18,18,18	0
3	ZN	D	702	1/1	0.73	0.11	-5.56	17,17,17,17	0
3	ZN	E	703	1/1	0.73	0.08	-10.12	17,17,17,17	0
7	SO4	K	707	5/5	0.78	0.32	-	53,54,58,71	0
7	SO4	C	709	5/5	0.35	0.57	-	55,55,63,82	0
5	1PE	K	705	12/16	0.37	0.38	-	29,41,46,47	0
5	1PE	A	706	12/16	-0.04	0.87	-	33,46,50,51	0
7	SO4	G	708	5/5	0.85	0.34	-	41,43,46,58	0
7	SO4	J	709	5/5	0.57	0.80	-	30,33,41,44	5
5	1PE	J	706	11/16	0.43	0.40	-	36,43,47,52	0
7	SO4	C	707	5/5	0.52	0.47	-	57,57,57,58	0
5	1PE	D	705	10/16	0.01	0.53	-	27,37,45,48	0
7	SO4	L	707	5/5	0.80	0.35	-	62,63,64,66	0
5	1PE	I	705	12/16	0.53	0.31	-	35,40,43,47	0
5	1PE	C	705	13/16	0.42	0.35	-	27,41,52,52	0
5	1PE	B	706	10/16	0.46	0.58	-	41,45,54,56	0
7	SO4	D	707	5/5	0.74	0.35	-	42,43,57,58	0
7	SO4	F	706	5/5	0.86	0.36	-	44,46,54,58	0
7	SO4	E	708	5/5	0.80	0.38	-	42,42,54,56	0
5	1PE	E	705	12/16	0.31	0.46	-	29,39,44,45	0
6	GOL	A	707	6/6	0.26	0.59	-	37,37,45,54	0
5	1PE	H	705	10/16	0.34	0.63	-	35,44,50,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	SO4	I	707	5/5	0.67	0.33	-	52,58,61,64	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.