



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 07:20 am 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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

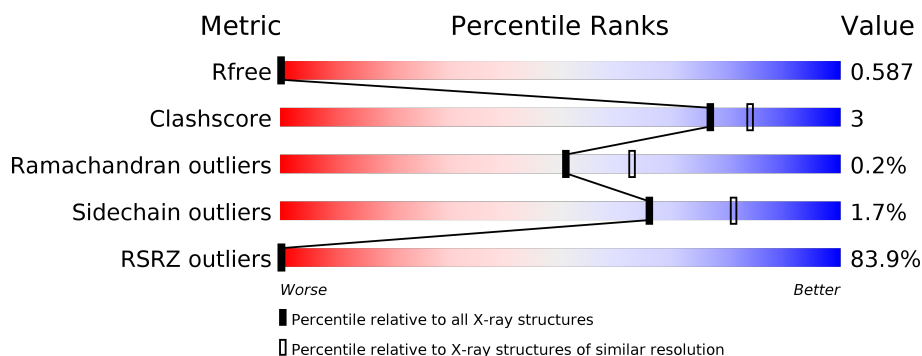
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (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 ≥ 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>88%</div> <div> <div></div> <div>92%</div> <div>8%</div> </div> </div>
1	B	519	<div> <div>84%</div> <div> <div></div> <div>89%</div> <div>10%</div> <div>•</div> </div> </div>
1	C	519	<div> <div>86%</div> <div> <div></div> <div>91%</div> <div>9%</div> </div> </div>
1	D	519	<div> <div>77%</div> <div> <div></div> <div>89%</div> <div>10%</div> <div>•</div> </div> </div>
1	E	519	<div> <div>82%</div> <div> <div></div> <div>90%</div> <div>8%</div> <div>•</div> </div> </div>
1	F	519	<div> <div>82%</div> <div> <div></div> <div>90%</div> <div>8%</div> <div>•</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	519	<div>87%</div> <div>90%</div> <div>10%</div>
1	H	519	<div>86%</div> <div>90%</div> <div>9%</div>
1	I	519	<div>84%</div> <div>92%</div> <div>7%</div>
1	J	519	<div>78%</div> <div>87%</div> <div>11%</div>
1	K	519	<div>83%</div> <div>92%</div> <div>6%</div>
1	L	519	<div>81%</div> <div>90%</div> <div>8%</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	711	-	-	-	X
7	SO4	A	712	-	-	X	X
7	SO4	C	708	-	-	-	X
7	SO4	C	710	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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:

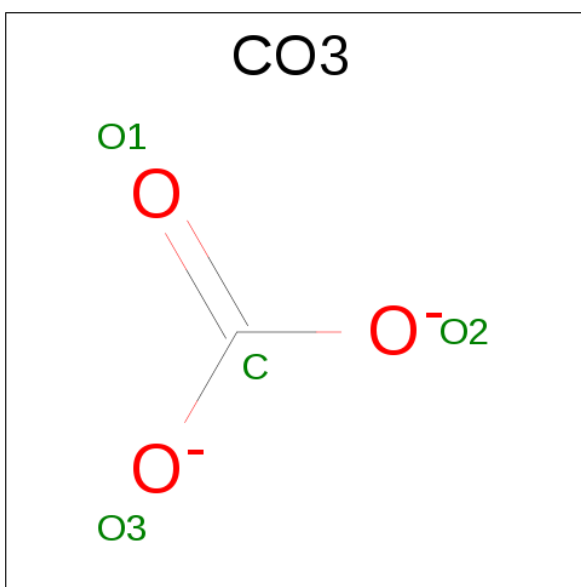
Chain	Residue	Modelled	Actual	Comment	Reference
A	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
A	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
A	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
B	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
B	515	GLN	ASN	engineered mutation	UNP A0A024V0B1

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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: CO₃).

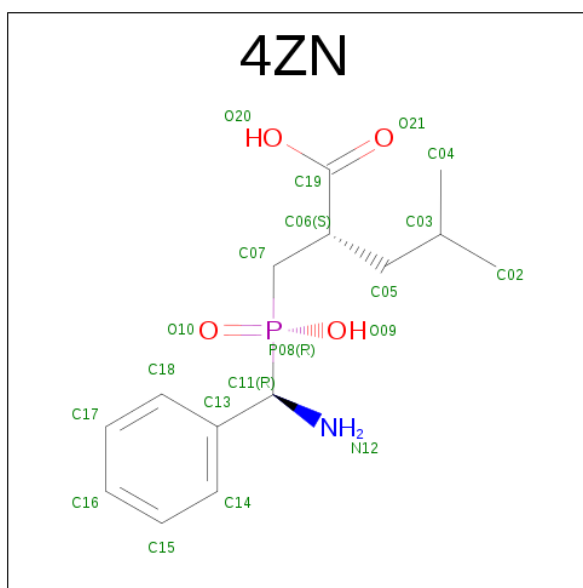


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	1	3		
2	B	1	Total	C	O	0	0
			4	1	3		
2	C	1	Total	C	O	0	0
			4	1	3		
2	D	1	Total	C	O	0	0
			4	1	3		
2	E	1	Total	C	O	0	0
			4	1	3		
2	F	1	Total	C	O	0	0
			4	1	3		
2	G	1	Total	C	O	0	0
			4	1	3		
2	H	1	Total	C	O	0	0
			4	1	3		
2	I	1	Total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

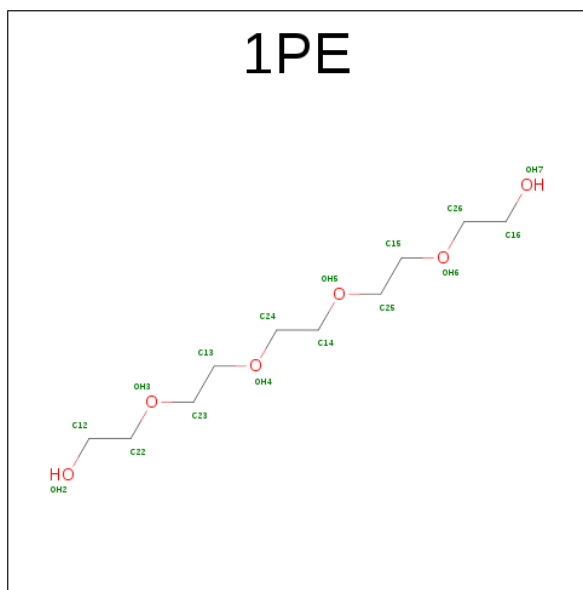
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	2	Total 2 Zn 2 2	0	0
3	J	2	Total 2 Zn 2 2	0	0
3	D	2	Total 2 Zn 2 2	0	0
3	K	2	Total 2 Zn 2 2	0	0
3	E	2	Total 2 Zn 2 2	0	0
3	H	2	Total 2 Zn 2 2	0	0
3	B	2	Total 2 Zn 2 2	0	0
3	I	2	Total 2 Zn 2 2	0	0
3	C	2	Total 2 Zn 2 2	0	0
3	A	2	Total 2 Zn 2 2	0	0
3	L	2	Total 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: C₁₄H₂₂NO₄P).



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: $C_{10}H_{22}O_6$).



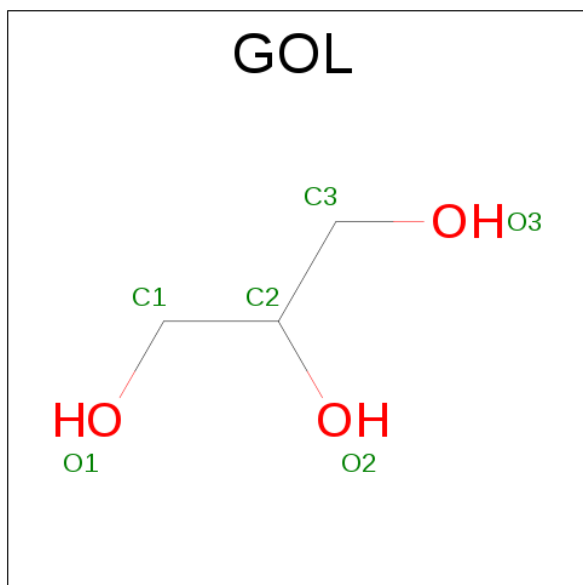
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 9 6 3	0	0
5	A	1	Total C O 12 8 4	0	0
5	B	1	Total C O 10 7 3	0	0
5	B	1	Total C O 10 7 3	0	0
5	C	1	Total C O 13 9 4	0	0
5	C	1	Total C O 9 6 3	0	0
5	D	1	Total C O 10 7 3	0	0
5	D	1	Total C O 10 7 3	0	0
5	E	1	Total C O 12 8 4	0	0
5	E	1	Total C O 12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

- Molecule 8 is water.

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

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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

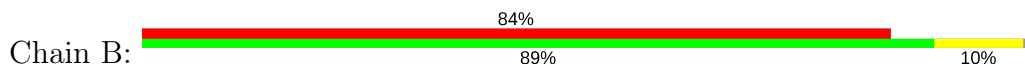
3 Residue-property plots

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

• Molecule 1: M17 family aminopeptidase



• Molecule 1: M17 family aminopeptidase



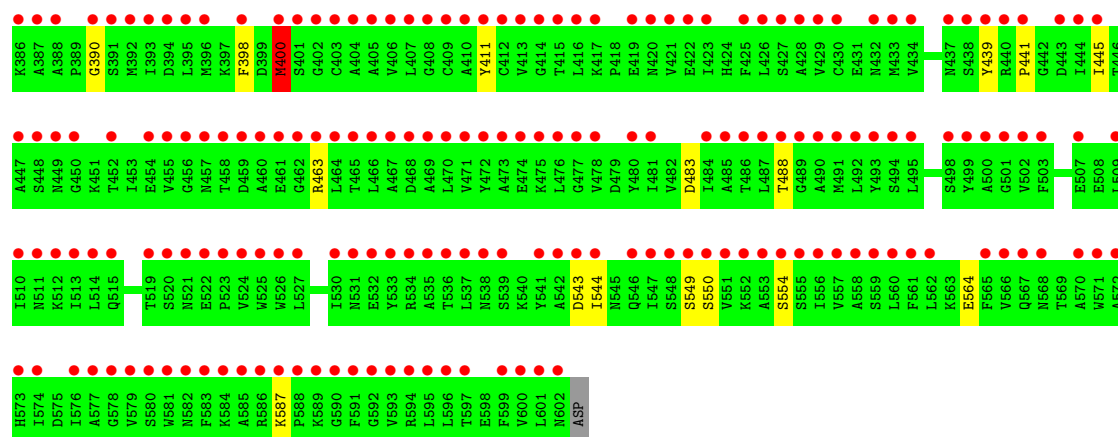
V579	S579	G456	I393	G329	L267	V206	S146	ALA
S580	K518	M457	D394	V330	G268	V207	K147	S86
S581	T519	T458	L395	K331	V269	L208	V148	S87
S582	S520	D459	K396	E332	G270	S209	N149	V88
S583	N521	A460	K397	L333	G271	L210	D150	P89
S584	S522	E461	F398	E334	N272	V211	K151	Q90
S585		G462	D399	E335	N273	L212	K152	
S586	W525	R463	M400	L336	A274	M213	V153	S93
S587	W526	L464	S401	K338	T276	L214	S154	L94
S588	L527	T465	G402	K339	T276	H215	E155	D95
S589	P528	K466	C403	G340	G277	D216	F156	P96
S590	L529	A467	A404	L340	K278	N217	L157	T97
S591	L530	D468	A405	K341	E279	K218	K158	S98
S592	N531	A469	V406	L342	E280	L219	D159	P99
S593	S532	L470	S432	K343		S220	E160	P100
S594	S533	V471	G408	V344	A284	K221	N161	I101
S595	S534	K472	C409	G345	R285	L222	M162	E102
S596	A535	A473	A410	K346	V286	T223	E163	Y103
S597	T536	K474	C411	G347	Y287	V224	K164	N104
S598	L537	E475	C412	S348	Y288	V225	F165	T105
S599	N538	L476	V413	K349	F289	F226	M166	P106
S600	S539	G477	G414	Y350	G290	E227	V167	I107
S601	K540	V478	T415	P351	T291	L228	K168	H108
S602	Y541	D479	L416	K352	Y292	N229	L169	D109
S603	A542	Y480	K417	L353	Y293	V230	G170	I110
S604	D543	L481	P418	F354	A294	D231	T171	K111
S605	L544	V482	E419	L355	S295	K232	S172	V112
S606	N545	D483	M420	H356	Q296	N233	K173	Q113
S607	O546	L484	V421	L357	L291	L234	H174	V114
S608	L547	A485	E422	T358	I298	F235	F175	Y115
S609	S548	T486	L423	G359	A299	K236	Y176	D116
S610	S549	L487	H424	K360	A300	F237	M177	I117
S611	S550	T488	F425	S361	S301	F238	F178	K118
S612	V551	G489	L426	K362	S302	L239	N179	G119
S613	K552	A490	S427	G363	N303	E240	D180	G120
S614	A553		A428	D364	Y304	T241	N181	C121
S615	S554	Y493	V429	V365	C305	L242	K182	N122
S616	S555	S494		K366	N306	F243	N183	V123
S617	L556	L495	M433		P307	Y244	S184	E124
S618	V557	G496	V434	T369	V308	E245	A185	G125
S619	A558	T497	S435	A370	S309	Y246	E186	E126
S620	S559	S498		L371	L310	M247	Y187	L127
S621	L560	Y499	S438	V372	S311	T248	G188	L128
S622	F561	A500	Y439	G373	N312	D249	Y189	I129
S623	L562	G501	R440	K374	A313	E250	G190	F130
S624	K563	V502	P441	G375	A314	R251	V191	L131
S625	E564	F503	G442	L376	V315	F252	C192	V132
S626	F565	G504	D443	T377	E316	K253	G193	N133
S627	V566	N505	L444	F378	L317	S254	S194	N134
S628	Q567	N506	I445		A318	T255	V195	P135
S629		E507	T446	G381	Q319	ASP	A196	G136
S630	A570	E508	A447	G382	K320	K257	D197	K137
S631	W571	L509	S448	Y383	L321	N258	L198	E138
S632	A572	I510	M449	N384	N322	V259	S199	N139
S633	H573	N511	G450	L385	L323	M260	E200	G140
S634	L574	K512	K451	K386	E324	M261	A201	P141
S635	D575	L513	T452	A387	K325	E262	D202	V142
S636	L576	L514	L453		K326	Y263	W203	K143
S637	A577	Q515	E454	S391	I327	L264	K204	I144
S638	S578	R516	V455	W292	L328		K205	G145

● Molecule 1: M17 family aminopeptidase

Chain C:



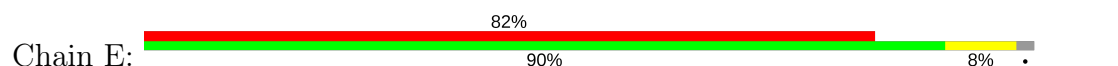
K326	K327	L328	G329	V330	K331	E332	L333	L333	E334	E335	L336	K337	K338	G339	A340	L341	L342	S343	G344	G345	K346	G347	S348	K349	F350	P351	K352	K353	F354	L355	H356	L357	K358	F359	K360	S361	K362	G363	D364	V365	K366	K367	K368	L369	S370	A371	L371	L372	G373	K374	G375	L376	T377	F378	D379	S380	G381	G382	K383	K384	L385
H266	L267	G268	V269	L270	L271	N272	N273	L274	D275	A276	L276	Z277	Z278	E279	E280	V281	E282	K283	A284	R285	V286	T287	V288	F289	G290	T291	V292	V293	A294	S295	Q296	L297	L298	A299	A300	P301	S302	N303	G304	V305	N306	P307	V308	S309	L310	S311	S312	A313	A314	V315	E316	L317	A318	Q319	K320	L321	N322	L323	K324	E325	
V206	L207	L208	S209	L210	V211	T212	M213	L214	H215	H216	N217	K218	L219	S220	K221	L222	T223	V224	V225	F226	E227	T228	N229	V230	D231	K232	N233	L234	F235	R236	F237	F238	L239	E240	T241	L242	F243	V244	E245	V246	N247	T248	D249	E250	R251	F252	K253	S254	T255	D256	K257	N258	V259	N260	M261	E262	V263	T264	V265		
S145	S146	K147	V148	M149	D150	V151	Q152	S153	S154	D155	F156	L157	K158	D159	M160	E162	E163	K164	F165	M166	V167	K168	L169	G170	T171	S172	K173	H174	F175	V176	M177	F178	N179	D180	M181	K182	N183	S184	V185	A186	V187	G188	V189	G190	V191	C192	G193	S194	V195	A196	D197	L198	S199	E200	A201	D202	M203	K204	R205		
ALA	S86	E87	V88	P89	Q90	V91	V92	S93	L94	D95	P96	L97	K98	I99	I100	I101	E102	I103	N104	T105	P106	I107	H108	D109	I110	K111	V112	Q113	V114	V115	D116	I117	K118	G119	G120	C121	N122	V123	E124	E125	G126	L127	T128	I129	F130	L131	C132	N133	P134	P135	G136	K137	E138	G139	A140	P141	V142	K143	T144		

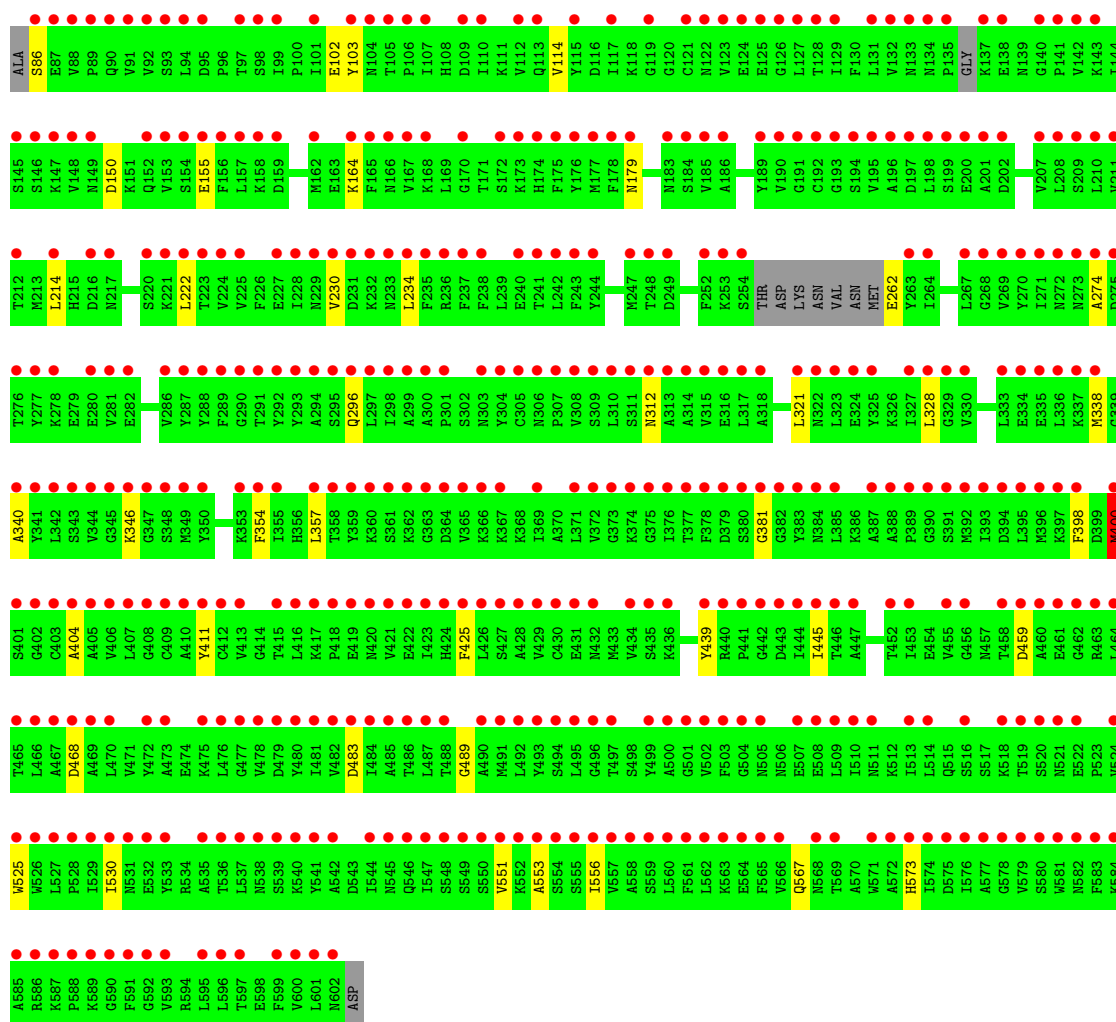


• Molecule 1: M17 family aminopeptidase



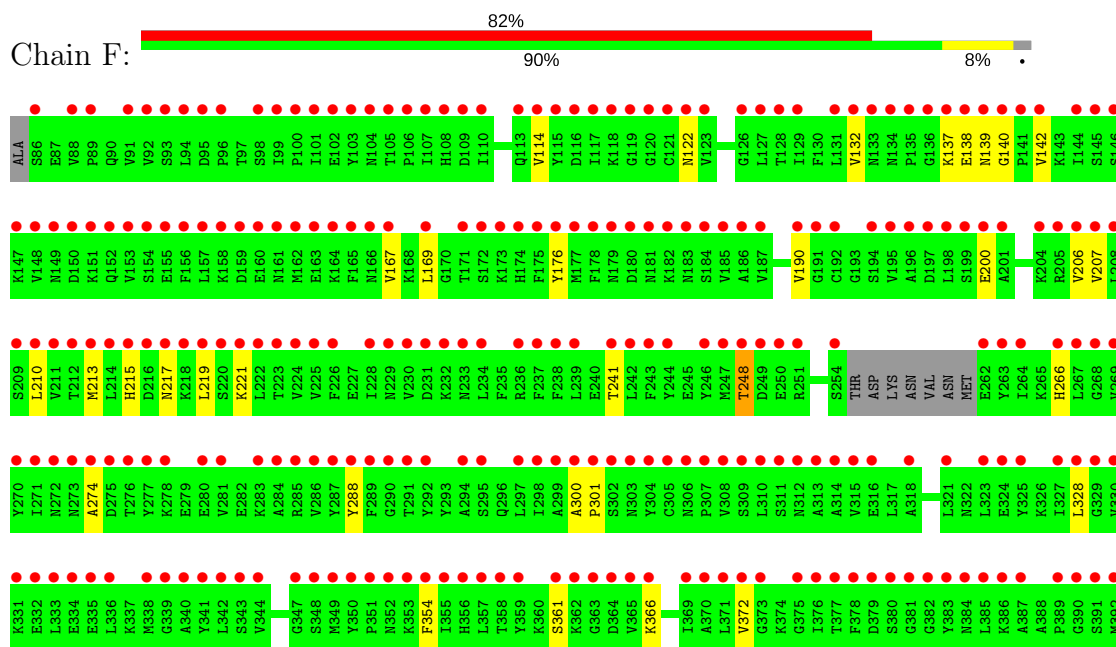
• Molecule 1: M17 family aminopeptidase

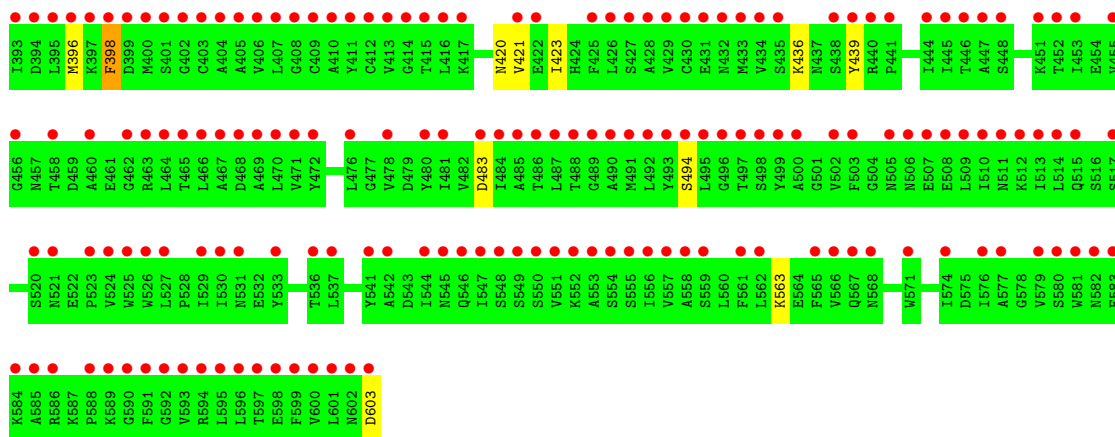




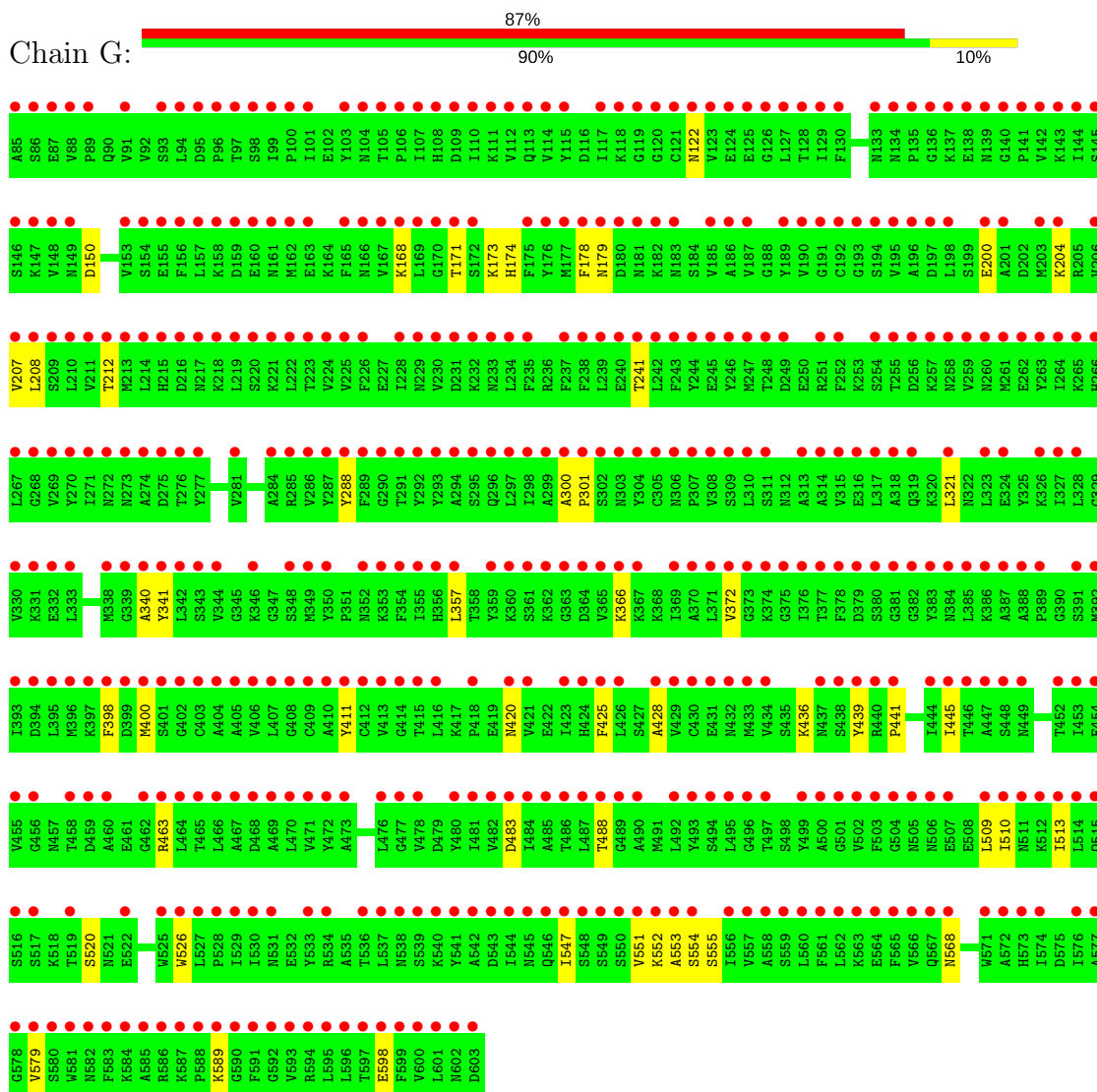
● Molecule 1: M17 family aminopeptidase

Chain F:

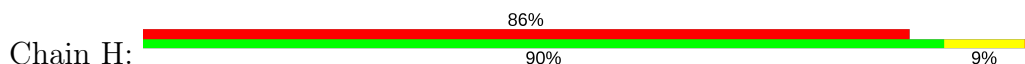




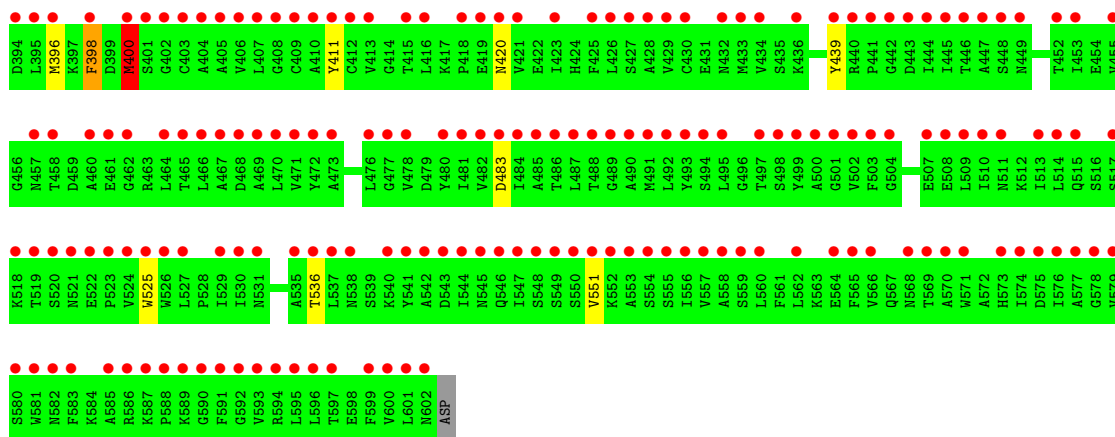
• Molecule 1: M17 family aminopeptidase



• Molecule 1: M17 family aminopeptidase



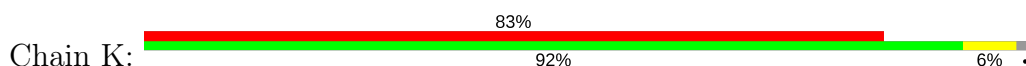




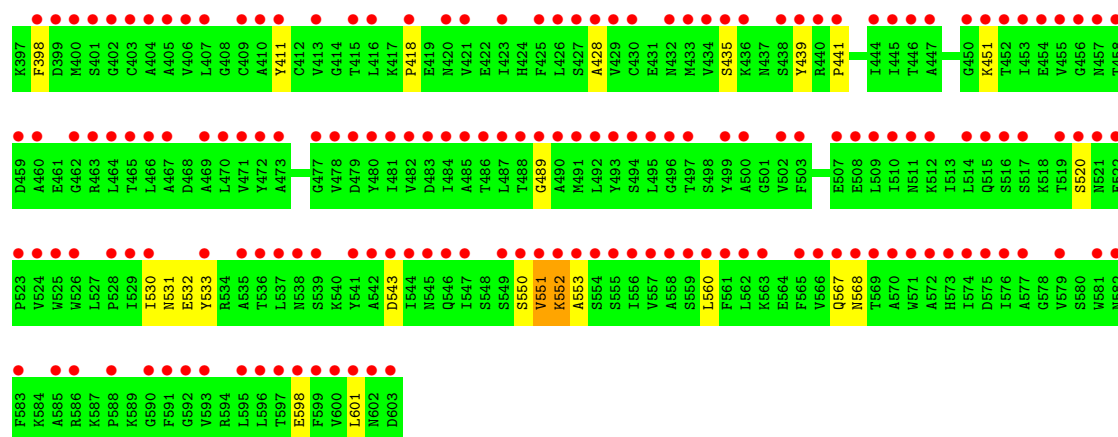
● Molecule 1: M17 family aminopeptidase



● Molecule 1: M17 family aminopeptidase







4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	0.98 (at 2.29Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.182 , 0.235 0.579 , 0.587	Depositor DCC
R_{free} test set	15699 reflections (5.24%)	DCC
Wilson B-factor (Å ²)	64.1	Xtriage
Anisotropy	0.534	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 24.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.39$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	50850	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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:E:114:VAL:HG12	1:E:274:ALA:HB1	1.81	0.61
1:J:282:GLU:OE1	8:J:801:HOH:O	2.16	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:E:411:TYR:HE1	5:E:706:1PE:H241	1.68	0.58
1:F:137:LYS:CB	1:F:140:GLY:H	2.16	0.58
1:H:138:GLU:C	1:H:139:ASN:HD22	2.07	0.58
1:D:214:LEU:HD21	1:D:222:LEU:HD22	1.85	0.58
1:K:328:LEU:HB2	1:K:354:PHE:HB3	1.84	0.58
1:L:551:VAL:HA	1:L:552:LYS:CB	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:230:VAL:HG12	1:H:234:LEU:HD23	1.85	0.57
1:L:137:LYS:CB	1:L:140:GLY:H	2.18	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:G:178:PHE:HZ	1:J:155:GLU:HG2	1.70	0.56
1:L:530:ILE:HA	5:L:705:1PE:H152	1.86	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:A:207:VAL:HG11	1:A:241:THR:HG22	1.87	0.56
1:L:232:LYS:NZ	1:L:279:GLU:OE2	2.31	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
5:J:705:1PE:H261	1:L:543:ASP:HB3	1.88	0.54
1:L:530:ILE:HG23	5:L:705:1PE:H141	1.89	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:328:LEU:HB2	1:A:354:PHE:HB3	1.90	0.54
1:A:489:GLY:N	4:A:704:4ZN:O21	2.35	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:H:103:TYR:CD2	5:H:705:1PE:H221	2.43	0.53
1:J:316:GLU:HG3	5:J:706:1PE:H262	1.89	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:H:413:VAL:HG11	1:H:423:ILE:HD13	1.92	0.52
1:J:132:VAL:HG11	1:J:144:ILE:HD13	1.91	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: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:L:567:GLN:HG3	8:L:986:HOH:O	2.10	0.51
1:A:208:LEU:O	1:A:212:THR:HG23	2.10	0.51
1:D:103:TYR:N	7:D:707:SO4:O3	2.30	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:F:122:ASN:HB3	8:F:966:HOH:O	2.11	0.50
1:G:178:PHE:CZ	1:J:155:GLU:HG2	2.46	0.50
1:E:346:LYS:NZ	8:E:808:HOH:O	2.33	0.50
1:G:122:ASN:ND2	5:G:706:1PE:H142	2.25	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:F:221:LYS:HG3	1:F:266:HIS:HB2	1.93	0.49
1:J:326:LYS:NZ	8:J:810:HOH:O	2.45	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:D:316:GLU:HG3	5:D:705:1PE:H221	1.95	0.49
1:L:139:ASN:N	8:L:810:HOH:O	2.43	0.49
1:A:174:HIS:HB3	1:D:175:PHE:CD2	2.48	0.49
1:A:150:ASP:OD2	1:A:179:ASN:HB2	2.12	0.49
1:G:463:ARG:NH1	7:G:711:SO4:O2	2.45	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:C:117:ILE:HD13	1:C:270:TYR:HB3	1.95	0.48
1:F:138:GLU:N	1:F:139:ASN:HA	2.27	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: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
1:I:230:VAL:HG12	1:I:234:LEU:HD23	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:B:255:THR:HA	8:B:829:HOH:O	2.13	0.47
1:B:341:TYR:CE1	1:B:428:ALA:HB1	2.49	0.47
1:D:381:GLY:HA2	1:D:459:ASP:OD1	2.14	0.47
1:F:366:LYS:HG3	1:F:420:ASN:HB3	1.96	0.47
1:H:340:ALA:HA	1:H:445:ILE:HD12	1.95	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:E:567:GLN:OE1	8:E:802:HOH:O	2.20	0.47
1:L:531:ASN:H	5:L:705:1PE:H152	1.78	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:A:321:LEU:HD11	1:A:411:TYR:HA	1.97	0.47
1:K:214:LEU:HD11	1:K:222:LEU:HD22	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: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
1:E:338:MET:CE	1:E:468:ASP:HB3	2.45	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:D:396:MET:SD	1:D:398:PHE:HE2	2.39	0.46
1:G:150:ASP:OD2	1:G:179:ASN:HB2	2.15	0.46
1:A:262:GLU:HA	8:A:835:HOH:O	2.16	0.46
1:G:174:HIS:HB3	1:J:175:PHE:CD2	2.51	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:B:460:ALA:HB3	1:B:546:GLN:NE2	2.31	0.45
1:I:321:LEU:HD11	1:I:411:TYR:HA	1.98	0.45
1:L:341:TYR:CE1	1:L:428:ALA:HB1	2.51	0.45
1:G:300:ALA:HA	1:G:301:PRO:HD3	1.83	0.45
1:G:372:VAL:O	1:G:483:ASP:HA	2.16	0.45
1:B:168:LYS:O	1:B:171:THR:HG22	2.16	0.45
1:G:357:LEU:HB2	1:G:425:PHE:HB2	1.97	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:C:216:ASP:HB3	8:E:916:HOH:O	2.17	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:J:411:TYR:CE1	5:J:707:1PE:H252	2.52	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:A:394:ASP:HA	1:C:441:PRO:HB2	1.99	0.44
1:D:343:SER:HA	1:D:346:LYS:HD3	1.98	0.44
1:H:283:LYS:HE2	1:H:287:TYR:CZ	2.52	0.44
1:H:506:ASN:O	1:H:510:ILE:HG12	2.18	0.44
1:L:551:VAL:HG12	1:L:553:ALA:H	1.82	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:J:232:LYS:HD2	1:J:276:THR:HG22	1.99	0.44
1:A:395:LEU:HD11	1:A:581:TRP:CG	2.52	0.44
1:H:106:PRO:HD2	1:H:247:MET:SD	2.58	0.44
1:H:509:LEU:O	1:H:513:ILE:HG12	2.18	0.44
1:I:320:LYS:HE2	5:I:705:1PE:H131	1.99	0.44
1:C:463:ARG:NH1	7:C:711:SO4:O3	2.48	0.44
1:D:326:LYS:HG2	1:D:328:LEU:HD12	2.00	0.44
1:G:509:LEU:O	1:G:513:ILE:HG12	2.18	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:J:302:SER:OG	1:J:378:PHE:HB2	2.18	0.44
1:H:321:LEU:HD11	1:H:411:TYR:HA	1.98	0.43
1:A:121:CYS:HA	1:A:270:TYR:CE2	2.53	0.43
1:L:137:LYS:C	1:L:139:ASN:HA	2.38	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:G:436:LYS:HE2	1:G:436:LYS:HB3	1.81	0.43
1:I:204:LYS:HE2	1:I:204:LYS:HB2	1.83	0.43
1:E:340:ALA:HA	1:E:445:ILE:HD12	2.00	0.43
1:E:357:LEU:HB2	1:E:425:PHE:HB2	1.99	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:L:533:TYR:HB2	1:L:560:LEU:HD11	1.99	0.43
5:L:705:1PE:H242	5:L:705:1PE:H252	1.83	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:C:230:VAL:HG12	1:C:234:LEU:HD23	2.01	0.43
1:G:168:LYS:HB3	1:G:171:THR:OG1	2.19	0.43
1:G:547:ILE:HB	7:G:711:SO4:O4	2.18	0.43
1:I:114:VAL:HG12	1:I:274:ALA:HB1	2.00	0.43
1:J:567:GLN:NE2	8:J:819:HOH:O	2.51	0.43
1:D:236:ARG:O	1:D:240:GLU:HG3	2.18	0.43
1:G:204:LYS:HB2	1:G:204:LYS:HE3	1.78	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:J:381:GLY:HA2	1:J:459:ASP:OD1	2.18	0.43
1:A:132:VAL:HG23	1:A:167:VAL:HG12	1.99	0.43
1:C:544:ILE:HD12	1:C:564:GLU:HG3	2.00	0.43
1:E:102:GLU:HG2	1:E:296:GLN:OE1	2.18	0.43
1:F:421:VAL:HG22	1:F:423:ILE:HG13	2.00	0.43
1:I:174:HIS:HB3	1:K:175:PHE:CD2	2.54	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:D:320:LYS:HE2	5:D:705:1PE:H231	2.01	0.43
1:K:366:LYS:HG3	1:K:420:ASN:HB3	2.01	0.43
1:G:510:ILE:HD13	1:G:526:TRP:NE1	2.34	0.43
1:H:350:TYR:HA	1:H:351:PRO:HD3	1.89	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:C:153:VAL:O	1:C:157:LEU:HG	2.19	0.42
1:G:122:ASN:HD21	5:G:707:1PE:H251	1.84	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:J:155:GLU:O	1:J:158:LYS:HG2	2.19	0.42
1:L:103:TYR:HB3	5:L:706:1PE:H252	2.01	0.42
1:E:400:MET:HE2	1:E:404:ALA:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:552:LYS:O	1:J:553:ALA:HB3	2.19	0.42
1:L:292:TYR:O	1:L:296:GLN:HG3	2.20	0.42
1:A:357:LEU:HB2	1:A:425:PHE:HB2	2.00	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:B:294:ALA:O	1:B:298:ILE:HG13	2.20	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:181:ASN:ND2	1:B:183:ASN:OD1	2.52	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: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:173:LYS:HD2	1:J:176:TYR:HE1	1.84	0.42
1:G:340:ALA:HA	1:G:445:ILE:HD12	2.01	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: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:I:150:ASP:OD2	1:I:179:ASN:HB2	2.20	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:C:135:PRO:HA	1:C:194:SER:O	2.19	0.41
1:J:551:VAL:HG12	1:J:552:LYS:O	2.20	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
4:C:704:4ZN:O10	4:C:704:4ZN:H20	2.20	0.41
1:D:300:ALA:HA	1:D:301:PRO:HD3	1.92	0.41
1:D:342:LEU:HA	1:D:342:LEU:HD23	1.89	0.41
1:E:150:ASP:OD2	1:E:179:ASN:HB2	2.21	0.41
1:L:418:PRO:HB3	1:L:601:LEU:HD12	2.03	0.41
1:B:287:TYR:CD2	1:B:594:ARG:HG2	2.56	0.41
1:B:372:VAL:O	1:B:483:ASP:HA	2.20	0.41
1:J:106:PRO:HD3	8:J:1001:HOH:O	2.20	0.41
1:J:294:ALA:O	1:J:298:ILE:HG13	2.20	0.41
1:C:488:THR:HG22	8:C:1002:HOH:O	2.21	0.41
1:J:214:LEU:HD11	1:J:222:LEU:HD22	2.02	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:F:396:MET:SD	1:F:398:PHE:HE2	2.44	0.41
1:H:138:GLU:O	1:H:194:SER:OG	2.39	0.41
1:B:383:TYR:HE1	1:B:438:SER:HB2	1.85	0.41
1:D:132:VAL:HG11	1:D:144:ILE:HD13	2.02	0.41
1:H:499:TYR:CD1	1:H:523:PRO:HB2	2.55	0.41
1:J:320:LYS:HB3	5:J:707:1PE:H242	2.02	0.41
1:G:551:VAL:O	1:G:552:LYS:HB2	2.21	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:I:400:MET:H	1:I:400:MET:HG3	1.27	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:J:372:VAL:O	1:J:483:ASP:HA	2.20	0.40
1:C:340:ALA:HA	1:C:445:ILE:HD12	2.02	0.40
1:D:210:LEU:HD12	1:D:213:MET:HE3	2.02	0.40
1:F:436:LYS:HB3	1:F:436:LYS:HE2	1.98	0.40
1:H:449:ASN:HD21	1:H:451:LYS:HD2	1.86	0.40
1:J:341:TYR:CE1	1:J:428:ALA:HB1	2.56	0.40
1:L:138:GLU:N	1:L:139:ASN:CA	2.83	0.40
1:B:235:PHE:O	1:B:238:PHE:HB3	2.20	0.40
1:D:364:ASP:O	1:D:420:ASN:HA	2.21	0.40
1:E:103:TYR:CD2	5:E:705:1PE:H132	2.56	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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	518/519 (100%)	501 (97%)	16 (3%)	1 (0%)	51	63
1	B	512/519 (99%)	495 (97%)	16 (3%)	1 (0%)	51	63
1	C	515/519 (99%)	499 (97%)	15 (3%)	1 (0%)	51	63
1	D	510/519 (98%)	496 (97%)	13 (2%)	1 (0%)	51	63
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%)	38	47
1	I	515/519 (99%)	505 (98%)	8 (2%)	2 (0%)	38	47
1	J	510/519 (98%)	496 (97%)	12 (2%)	2 (0%)	38	47
1	K	503/519 (97%)	490 (97%)	10 (2%)	3 (1%)	28	34
1	L	507/519 (98%)	491 (97%)	14 (3%)	2 (0%)	38	47
All	All	6130/6228 (98%)	5959 (97%)	156 (2%)	15 (0%)	51	63

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%)	71	85
1	B	407/447 (91%)	403 (99%)	4 (1%)	80	90
1	C	418/447 (94%)	406 (97%)	12 (3%)	48	64
1	D	413/447 (92%)	405 (98%)	8 (2%)	62	78
1	E	413/447 (92%)	410 (99%)	3 (1%)	87	94
1	F	402/447 (90%)	391 (97%)	11 (3%)	50	67
1	G	422/447 (94%)	415 (98%)	7 (2%)	66	81
1	H	406/447 (91%)	397 (98%)	9 (2%)	57	74
1	I	420/447 (94%)	414 (99%)	6 (1%)	71	85
1	J	414/447 (93%)	408 (99%)	6 (1%)	71	85
1	K	410/447 (92%)	406 (99%)	4 (1%)	80	90
1	L	400/447 (90%)	394 (98%)	6 (2%)	70	83
All	All	4948/5364 (92%)	4866 (98%)	82 (2%)	66	81

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	14,22,28	1.45	3 (21%)
5	1PE	A	705	-	8,8,15	0.75	0	7,7,14	0.34	0
5	1PE	A	706	-	11,11,15	0.79	0	10,10,14	0.33	0
6	GOL	A	707	-	5,5,5	0.43	0	5,5,5	0.20	0
7	SO4	A	708	-	4,4,4	0.21	0	6,6,6	0.23	0
7	SO4	A	709	-	4,4,4	0.23	0	6,6,6	0.10	0
7	SO4	A	710	-	4,4,4	0.25	0	6,6,6	0.34	0
7	SO4	A	711	-	4,4,4	0.25	0	6,6,6	0.21	0
7	SO4	A	712	-	4,4,4	0.23	0	6,6,6	0.56	0
2	CO3	B	701	-	0,3,3	0.00	-	0,3,3	0.00	-
4	4ZN	B	704	3	10,16,20	0.76	0	14,22,28	2.93	6 (42%)
5	1PE	B	705	-	9,9,15	0.70	0	8,8,14	0.38	0
5	1PE	B	706	-	9,9,15	0.72	0	8,8,14	0.46	0
7	SO4	B	707	-	4,4,4	0.16	0	6,6,6	0.27	0
2	CO3	C	701	-	0,3,3	0.00	-	0,3,3	0.00	-
4	4ZN	C	704	3	10,16,20	1.50	1 (10%)	14,22,28	0.69	0
5	1PE	C	705	-	12,12,15	0.80	0	11,11,14	0.55	0
5	1PE	C	706	-	8,8,15	0.78	0	7,7,14	0.30	0
7	SO4	C	707	-	4,4,4	0.15	0	6,6,6	0.11	0
7	SO4	C	708	-	4,4,4	0.24	0	6,6,6	0.27	0
7	SO4	C	709	-	4,4,4	0.32	0	6,6,6	0.31	0
7	SO4	C	710	-	4,4,4	0.33	0	6,6,6	0.24	0
7	SO4	C	711	-	4,4,4	0.30	0	6,6,6	0.37	0
2	CO3	D	701	-	0,3,3	0.00	-	0,3,3	0.00	-
4	4ZN	D	704	3	14,20,20	1.41	2 (14%)	18,28,28	2.35	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	0.82	0	8,8,14	0.48	0
5	1PE	D	706	-	9,9,15	0.76	0	8,8,14	0.34	0
7	SO4	D	707	-	4,4,4	0.25	0	6,6,6	0.24	0
2	CO3	E	701	-	0,3,3	0.00	-	0,3,3	0.00	-
4	4ZN	E	704	3	14,20,20	0.71	1 (7%)	18,28,28	2.17	6 (33%)
5	1PE	E	705	-	11,11,15	0.83	0	10,10,14	0.38	0
5	1PE	E	706	-	11,11,15	0.71	0	10,10,14	0.31	0
7	SO4	E	707	-	4,4,4	0.17	0	6,6,6	0.14	0
7	SO4	E	708	-	4,4,4	0.19	0	6,6,6	0.23	0
7	SO4	E	709	-	4,4,4	0.29	0	6,6,6	0.11	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	14,22,28	1.41	2 (14%)
5	1PE	F	705	-	9,9,15	0.69	0	8,8,14	0.38	0
7	SO4	F	706	-	4,4,4	0.25	0	6,6,6	0.15	0
7	SO4	F	707	-	4,4,4	0.28	0	6,6,6	0.13	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	14,22,28	1.54	3 (21%)
5	1PE	G	705	-	8,8,15	0.71	0	7,7,14	0.33	0
5	1PE	G	706	-	5,5,15	0.61	0	4,4,14	0.58	0
5	1PE	G	707	-	5,5,15	0.69	0	4,4,14	0.43	0
7	SO4	G	708	-	4,4,4	0.22	0	6,6,6	0.12	0
7	SO4	G	709	-	4,4,4	0.15	0	6,6,6	0.22	0
7	SO4	G	710	-	4,4,4	0.25	0	6,6,6	0.15	0
7	SO4	G	711	-	4,4,4	0.18	0	6,6,6	0.50	0
2	CO3	H	701	-	0,3,3	0.00	-	0,3,3	0.00	-
4	4ZN	H	704	3	10,16,20	1.76	2 (20%)	14,22,28	1.08	2 (14%)
5	1PE	H	705	-	9,9,15	0.76	0	8,8,14	0.26	0
5	1PE	H	706	-	9,9,15	0.75	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	8,12,20	1.57	1 (12%)	12,17,28	1.73	1 (8%)
5	1PE	I	705	-	11,11,15	0.76	0	10,10,14	0.40	0
5	1PE	I	706	-	10,10,15	0.71	0	9,9,14	0.46	0
7	SO4	I	707	-	4,4,4	0.17	0	6,6,6	0.19	0
7	SO4	I	708	-	4,4,4	0.18	0	6,6,6	0.10	0
2	CO3	J	701	-	0,3,3	0.00	-	0,3,3	0.00	-
4	4ZN	J	704	3	10,16,20	1.47	1 (10%)	14,22,28	1.03	1 (7%)
5	1PE	J	705	-	10,10,15	0.69	0	9,9,14	0.40	0
5	1PE	J	706	-	10,10,15	0.72	0	9,9,14	0.46	0
5	1PE	J	707	-	9,9,15	0.61	0	8,8,14	0.32	0
7	SO4	J	708	-	4,4,4	0.14	0	6,6,6	0.30	0
7	SO4	J	709	-	4,4,4	0.15	0	6,6,6	0.12	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	0.81	1 (9%)	15,19,28	1.43	2 (13%)
5	1PE	K	705	-	11,11,15	0.72	0	10,10,14	0.25	0
5	1PE	K	706	-	11,11,15	0.74	0	10,10,14	0.45	0
7	SO4	K	707	-	4,4,4	0.21	0	6,6,6	0.12	0
7	SO4	K	708	-	4,4,4	0.17	0	6,6,6	0.25	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	14,22,28	1.00	0
5	1PE	L	705	-	6,6,15	0.72	0	5,5,14	0.36	0
5	1PE	L	706	-	9,9,15	0.63	0	8,8,14	0.41	0
7	SO4	L	707	-	4,4,4	0.16	0	6,6,6	0.16	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 (9) 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	I	704	4ZN	P08-O10	4.02	1.57	1.50
4	D	704	4ZN	P08-O10	4.26	1.57	1.49
4	C	704	4ZN	P08-O10	4.39	1.58	1.49
4	J	704	4ZN	P08-O10	4.55	1.58	1.49
4	H	704	4ZN	P08-O10	4.78	1.58	1.49

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	704	4ZN	O09-P08-O10	-5.42	107.35	113.96
4	B	704	4ZN	O10-P08-C11	-3.57	104.65	111.45
4	E	704	4ZN	O10-P08-C11	-3.19	105.38	111.45
4	G	704	4ZN	O10-P08-C11	-3.11	105.52	111.45
4	D	704	4ZN	C13-C11-N12	-2.91	104.80	112.74
4	A	704	4ZN	O10-P08-C11	-2.80	106.12	111.45
4	D	704	4ZN	C18-C13-C11	-2.71	117.83	120.72
4	B	704	4ZN	C18-C13-C11	-2.63	117.92	120.72
4	K	704	4ZN	O10-P08-C11	-2.54	106.62	111.45
4	E	704	4ZN	C13-C11-N12	-2.52	105.85	112.74
4	A	704	4ZN	C07-C06-C19	-2.45	106.93	111.54
4	H	704	4ZN	C13-C11-N12	-2.13	106.92	112.74
4	F	704	4ZN	C13-C11-N12	-2.08	107.04	112.74
4	E	704	4ZN	C18-C13-C11	-2.03	118.56	120.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	704	4ZN	O09-P08-C11	2.02	111.31	107.08
4	B	704	4ZN	C14-C13-C11	2.03	122.89	120.72
4	J	704	4ZN	C07-P08-C11	2.18	111.94	106.82
4	K	704	4ZN	O09-P08-C11	2.45	112.21	107.08
4	H	704	4ZN	C07-P08-C11	2.46	112.61	106.82
4	A	704	4ZN	O09-P08-C11	2.73	112.80	107.08
4	G	704	4ZN	P08-C11-C13	2.79	116.73	111.74
4	F	704	4ZN	P08-C11-C13	3.05	117.18	111.74
4	D	704	4ZN	C06-C05-C03	3.38	122.74	115.76
4	E	704	4ZN	P08-C11-C13	3.67	118.30	111.74
4	B	704	4ZN	P08-C11-C13	3.77	118.47	111.74
4	E	704	4ZN	C07-P08-C11	4.20	116.25	106.85
4	E	704	4ZN	C06-C05-C03	4.64	125.35	115.76
4	D	704	4ZN	P08-C11-C13	5.16	120.95	111.74
4	D	704	4ZN	C07-P08-C11	5.55	119.27	106.85
4	B	704	4ZN	C07-C06-C19	5.64	122.13	111.54
4	B	704	4ZN	C07-P08-C11	7.03	123.35	106.82

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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	707	1PE	1	0
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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	519/519 (100%)	3.50	458 (88%) 0 0	14, 23, 41, 61	3 (0%)
1	B	516/519 (99%)	3.61	435 (84%) 0 0	13, 25, 56, 73	5 (0%)
1	C	517/519 (99%)	3.28	446 (86%) 0 0	13, 23, 43, 60	3 (0%)
1	D	514/519 (99%)	2.98	400 (77%) 0 0	14, 23, 38, 58	1 (0%)
1	E	509/519 (98%)	3.18	425 (83%) 0 0	13, 22, 35, 48	2 (0%)
1	F	511/519 (98%)	3.48	426 (83%) 0 0	16, 26, 54, 71	9 (1%)
1	G	519/519 (100%)	3.41	449 (86%) 0 0	14, 23, 40, 55	5 (0%)
1	H	517/519 (99%)	3.67	448 (86%) 0 0	14, 27, 58, 73	5 (0%)
1	I	517/519 (99%)	3.32	434 (83%) 0 0	13, 25, 46, 63	5 (0%)
1	J	514/519 (99%)	3.09	404 (78%) 0 0	13, 23, 39, 55	6 (1%)
1	K	509/519 (98%)	3.23	433 (85%) 0 0	15, 23, 37, 62	3 (0%)
1	L	511/519 (98%)	3.48	421 (82%) 0 0	15, 25, 52, 62	6 (1%)
All	All	6173/6228 (99%)	3.35	5179 (83%) 0 0	13, 24, 49, 73	53 (0%)

All (5179) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	136	GLY	13.9
1	F	121	CYS	12.8
1	J	603	ASP	12.3
1	L	197	ASP	11.4
1	F	138	GLU	11.2
1	J	136	GLY	11.0
1	H	261	MET	10.9
1	B	272	ASN	10.8
1	L	363	GLY	10.6
1	H	255	THR	10.6
1	D	85	ALA	10.6

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Mol	Chain	Res	Type	RSRZ
1	L	119	GLY	10.4
1	L	138	GLU	10.3
1	F	197	ASP	10.0
1	H	135	PRO	9.8
1	B	121	CYS	9.8
1	A	363	GLY	9.6
1	B	202	ASP	9.5
1	L	147	LYS	9.5
1	G	551	VAL	9.5
1	B	150	ASP	9.5
1	L	153	VAL	9.3
1	D	136	GLY	9.3
1	F	267	LEU	9.2
1	B	228	ILE	9.0
1	H	144	ILE	8.9
1	B	157	LEU	8.9
1	L	494	SER	8.9
1	B	600	VAL	8.8
1	B	261	MET	8.7
1	I	576	ILE	8.6
1	F	179	ASN	8.6
1	D	603	ASP	8.6
1	H	597	THR	8.6
1	F	88	VAL	8.5
1	F	180	ASP	8.5
1	F	178	PHE	8.4
1	F	549	SER	8.4
1	I	230	VAL	8.4
1	H	603	ASP	8.4
1	L	159	ASP	8.4
1	K	99	ILE	8.4
1	A	603	ASP	8.4
1	C	136	GLY	8.4
1	J	363	GLY	8.3
1	H	202	ASP	8.3
1	H	260	ASN	8.3
1	H	257	LYS	8.3
1	E	549	SER	8.3
1	H	185	VAL	8.2
1	C	365	VAL	8.2
1	A	550	SER	8.2
1	G	550	SER	8.1

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Mol	Chain	Res	Type	RSRZ
1	B	118	LYS	8.1
1	I	510	ILE	8.1
1	L	134	ASN	8.0
1	B	144	ILE	8.0
1	I	121	CYS	8.0
1	A	600	VAL	8.0
1	F	185	VAL	7.9
1	B	123	VAL	7.9
1	D	198	LEU	7.9
1	L	161	ASN	7.9
1	F	159	ASP	7.9
1	C	134	ASN	7.9
1	I	117	ILE	7.8
1	D	196	ALA	7.8
1	H	189	TYR	7.8
1	A	85	ALA	7.8
1	B	143	LYS	7.8
1	K	576	ILE	7.8
1	H	276	THR	7.7
1	I	565	PHE	7.7
1	L	121	CYS	7.7
1	B	149	ASN	7.6
1	L	135	PRO	7.6
1	E	576	ILE	7.6
1	B	557	VAL	7.6
1	H	165	PHE	7.6
1	J	300	ALA	7.6
1	B	271	ILE	7.6
1	A	362	LYS	7.6
1	B	255	THR	7.5
1	F	145	SER	7.5
1	H	275	ASP	7.5
1	L	364	ASP	7.5
1	K	558	ALA	7.4
1	B	403	CYS	7.4
1	H	239	LEU	7.4
1	B	165	PHE	7.4
1	B	195	VAL	7.4
1	H	549	SER	7.4
1	E	596	LEU	7.4
1	F	579	VAL	7.4
1	B	363	GLY	7.4

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Mol	Chain	Res	Type	RSRZ
1	A	260	ASN	7.4
1	F	141	PRO	7.3
1	D	547	ILE	7.3
1	J	196	ALA	7.3
1	B	161	ASN	7.3
1	H	159	ASP	7.3
1	B	132	VAL	7.3
1	G	557	VAL	7.3
1	J	123	VAL	7.3
1	I	140	GLY	7.3
1	L	183	ASN	7.3
1	F	434	VAL	7.2
1	H	225	VAL	7.2
1	J	178	PHE	7.2
1	H	157	LEU	7.2
1	F	377	THR	7.2
1	H	122	ASN	7.2
1	H	117	ILE	7.2
1	B	136	GLY	7.2
1	J	184	SER	7.2
1	C	194	SER	7.1
1	B	556	ILE	7.1
1	F	364	ASP	7.1
1	H	333	LEU	7.1
1	A	398	PHE	7.1
1	L	179	ASN	7.1
1	B	192	CYS	7.1
1	A	295	SER	7.1
1	F	183	ASN	7.1
1	J	183	ASN	7.1
1	J	600	VAL	7.1
1	A	130	PHE	7.1
1	B	548	SER	7.0
1	B	122	ASN	7.0
1	F	122	ASN	7.0
1	G	85	ALA	7.0
1	F	123	VAL	7.0
1	F	135	PRO	7.0
1	B	131	LEU	7.0
1	K	406	VAL	7.0
1	L	148	VAL	7.0
1	G	261	MET	6.9

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Mol	Chain	Res	Type	RSRZ
1	L	177	MET	6.9
1	H	217	ASN	6.9
1	B	549	SER	6.9
1	H	143	LYS	6.9
1	E	395	LEU	6.9
1	K	305	CYS	6.9
1	K	551	VAL	6.9
1	L	434	VAL	6.9
1	K	419	GLU	6.9
1	E	294	ALA	6.9
1	E	391	SER	6.9
1	G	267	LEU	6.9
1	H	234	LEU	6.9
1	H	180	ASP	6.9
1	H	365	VAL	6.9
1	L	156	PHE	6.9
1	L	144	ILE	6.9
1	H	141	PRO	6.9
1	H	155	GLU	6.9
1	L	550	SER	6.9
1	H	134	ASN	6.9
1	G	600	VAL	6.8
1	B	229	ASN	6.8
1	H	187	VAL	6.8
1	C	163	GLU	6.8
1	B	153	VAL	6.8
1	C	88	VAL	6.8
1	L	487	LEU	6.8
1	G	342	LEU	6.7
1	E	148	VAL	6.7
1	H	132	VAL	6.7
1	H	486	THR	6.7
1	I	135	PRO	6.7
1	H	154	SER	6.7
1	H	123	VAL	6.7
1	A	576	ILE	6.7
1	F	155	GLU	6.7
1	A	256	ASP	6.7
1	F	268	GLY	6.7
1	J	471	VAL	6.7
1	B	234	LEU	6.7
1	A	305	CYS	6.6

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Mol	Chain	Res	Type	RSRZ
1	C	403	CYS	6.6
1	B	446	THR	6.6
1	B	197	ASP	6.6
1	L	322	ASN	6.6
1	J	194	SER	6.6
1	I	292	TYR	6.6
1	F	272	ASN	6.6
1	L	145	SER	6.6
1	H	201	ALA	6.6
1	K	196	ALA	6.6
1	C	132	VAL	6.6
1	G	365	VAL	6.6
1	L	155	GLU	6.6
1	B	135	PRO	6.5
1	I	146	SER	6.5
1	G	286	VAL	6.5
1	L	178	PHE	6.5
1	F	600	VAL	6.5
1	E	466	LEU	6.5
1	C	602	ASN	6.5
1	I	294	ALA	6.5
1	H	145	SER	6.5
1	A	119	GLY	6.5
1	E	484	ILE	6.5
1	C	297	LEU	6.5
1	I	466	LEU	6.5
1	K	385	LEU	6.5
1	L	603	ASP	6.5
1	B	133	ASN	6.5
1	E	372	VAL	6.5
1	L	234	LEU	6.5
1	E	409	CYS	6.5
1	C	180	ASP	6.5
1	B	145	SER	6.4
1	F	110	ILE	6.4
1	I	144	ILE	6.4
1	I	407	LEU	6.4
1	K	509	LEU	6.4
1	G	585	ALA	6.4
1	B	301	PRO	6.4
1	C	310	LEU	6.4
1	K	210	LEU	6.4

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Mol	Chain	Res	Type	RSRZ
1	B	269	VAL	6.4
1	B	156	PHE	6.4
1	I	200	GLU	6.4
1	B	294	ALA	6.4
1	I	387	ALA	6.4
1	H	409	CYS	6.4
1	G	178	PHE	6.4
1	G	549	SER	6.4
1	D	576	ILE	6.4
1	C	407	LEU	6.4
1	F	184	SER	6.4
1	G	562	LEU	6.4
1	L	485	ALA	6.3
1	B	476	LEU	6.3
1	C	576	ILE	6.3
1	J	161	ASN	6.3
1	L	122	ASN	6.3
1	A	277	TYR	6.3
1	A	99	ILE	6.3
1	A	294	ALA	6.3
1	B	274	ALA	6.3
1	A	194	SER	6.3
1	I	93	SER	6.3
1	L	239	LEU	6.3
1	F	342	LEU	6.3
1	H	150	ASP	6.3
1	I	542	ALA	6.3
1	H	138	GLU	6.3
1	E	376	ILE	6.3
1	F	117	ILE	6.3
1	F	142	VAL	6.3
1	F	487	LEU	6.2
1	G	104	ASN	6.2
1	A	485	ALA	6.2
1	D	537	LEU	6.2
1	F	106	PRO	6.2
1	F	144	ILE	6.2
1	I	579	VAL	6.2
1	L	230	VAL	6.2
1	B	226	PHE	6.2
1	H	137	LYS	6.2
1	B	134	ASN	6.2

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Mol	Chain	Res	Type	RSRZ
1	B	166	ASN	6.2
1	F	149	ASN	6.2
1	J	269	VAL	6.2
1	L	410	ALA	6.2
1	F	153	VAL	6.2
1	J	298	ILE	6.2
1	K	510	ILE	6.2
1	A	526	TRP	6.2
1	B	93	SER	6.2
1	F	157	LEU	6.2
1	F	270	TYR	6.2
1	G	246	TYR	6.2
1	K	595	LEU	6.2
1	J	396	MET	6.1
1	E	601	LEU	6.1
1	C	117	ILE	6.1
1	L	176	TYR	6.1
1	F	150	ASP	6.1
1	A	487	LEU	6.1
1	G	537	LEU	6.1
1	B	277	TYR	6.1
1	G	211	VAL	6.1
1	F	181	ASN	6.1
1	H	476	LEU	6.1
1	I	214	LEU	6.1
1	B	416	LEU	6.1
1	A	572	ALA	6.1
1	K	185	VAL	6.1
1	G	289	PHE	6.1
1	H	130	PHE	6.1
1	L	165	PHE	6.1
1	B	558	ALA	6.0
1	A	117	ILE	6.0
1	C	144	ILE	6.0
1	B	154	SER	6.0
1	C	211	VAL	6.0
1	C	406	VAL	6.0
1	I	138	GLU	6.0
1	G	398	PHE	6.0
1	B	336	LEU	6.0
1	B	199	SER	6.0
1	G	391	SER	6.0

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Mol	Chain	Res	Type	RSRZ
1	A	557	VAL	6.0
1	J	406	VAL	6.0
1	F	398	PHE	6.0
1	G	363	GLY	6.0
1	B	184	SER	6.0
1	B	467	ALA	6.0
1	H	146	SER	6.0
1	J	576	ILE	6.0
1	B	148	VAL	6.0
1	H	230	VAL	6.0
1	J	148	VAL	6.0
1	E	289	PHE	6.0
1	G	467	ALA	6.0
1	D	305	CYS	6.0
1	K	376	ILE	6.0
1	L	99	ILE	6.0
1	H	269	VAL	6.0
1	I	202	ASP	6.0
1	L	254	SER	6.0
1	K	601	LEU	6.0
1	I	272	ASN	5.9
1	F	148	VAL	5.9
1	J	308	VAL	5.9
1	C	145	SER	5.9
1	L	323	LEU	5.9
1	B	162	MET	5.9
1	H	175	PHE	5.9
1	K	410	ALA	5.9
1	E	420	ASN	5.9
1	A	310	LEU	5.9
1	K	400	MET	5.9
1	L	141	PRO	5.9
1	D	426	LEU	5.9
1	J	547	ILE	5.9
1	C	551	VAL	5.9
1	I	194	SER	5.9
1	B	181	ASN	5.9
1	D	389	PRO	5.9
1	E	274	ALA	5.9
1	F	577	ALA	5.9
1	G	242	LEU	5.9
1	K	395	LEU	5.9

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Mol	Chain	Res	Type	RSRZ
1	B	146	SER	5.9
1	L	452	THR	5.9
1	B	260	ASN	5.9
1	F	114	VAL	5.9
1	H	392	MET	5.9
1	G	404	ALA	5.9
1	A	242	LEU	5.9
1	A	281	VAL	5.8
1	E	551	VAL	5.8
1	H	178	PHE	5.8
1	B	276	THR	5.8
1	C	363	GLY	5.8
1	F	151	LYS	5.8
1	H	423	ILE	5.8
1	E	308	VAL	5.8
1	A	601	LEU	5.8
1	I	385	LEU	5.8
1	E	600	VAL	5.8
1	K	364	ASP	5.8
1	A	110	ILE	5.8
1	F	601	LEU	5.8
1	H	121	CYS	5.8
1	I	469	ALA	5.8
1	A	222	LEU	5.8
1	F	492	LEU	5.8
1	F	446	THR	5.8
1	F	376	ILE	5.8
1	L	544	ILE	5.8
1	H	254	SER	5.8
1	L	336	LEU	5.7
1	L	492	LEU	5.7
1	I	393	ILE	5.7
1	E	490	ALA	5.7
1	B	185	VAL	5.7
1	L	142	VAL	5.7
1	F	152	GLN	5.7
1	H	136	GLY	5.7
1	A	259	VAL	5.7
1	B	112	VAL	5.7
1	F	195	VAL	5.7
1	A	255	THR	5.7
1	B	175	PHE	5.7

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Mol	Chain	Res	Type	RSRZ
1	C	127	LEU	5.7
1	L	180	ASP	5.7
1	A	318	ALA	5.7
1	K	500	ALA	5.7
1	I	260	ASN	5.7
1	H	569	THR	5.7
1	B	127	LEU	5.7
1	C	93	SER	5.7
1	E	396	MET	5.7
1	F	484	ILE	5.7
1	A	395	LEU	5.7
1	D	362	LYS	5.7
1	H	163	GLU	5.7
1	C	553	ALA	5.7
1	L	511	ASN	5.7
1	A	455	VAL	5.7
1	C	230	VAL	5.7
1	I	259	VAL	5.7
1	B	119	GLY	5.7
1	D	511	ASN	5.7
1	E	547	ILE	5.6
1	B	315	VAL	5.6
1	F	478	VAL	5.6
1	K	365	VAL	5.6
1	L	88	VAL	5.6
1	K	375	GLY	5.6
1	A	267	LEU	5.6
1	D	122	ASN	5.6
1	H	151	LYS	5.6
1	E	410	ALA	5.6
1	G	603	ASP	5.6
1	A	444	ILE	5.6
1	A	549	SER	5.6
1	B	579	VAL	5.6
1	D	455	VAL	5.6
1	H	128	THR	5.6
1	F	229	ASN	5.6
1	K	466	LEU	5.6
1	K	560	LEU	5.6
1	B	196	ALA	5.6
1	F	441	PRO	5.6
1	B	205	ARG	5.6

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Mol	Chain	Res	Type	RSRZ
1	L	117	ILE	5.6
1	A	311	SER	5.6
1	A	159	ASP	5.6
1	D	219	LEU	5.6
1	G	317	LEU	5.6
1	H	416	LEU	5.6
1	L	216	ASP	5.6
1	H	158	LYS	5.6
1	J	228	ILE	5.6
1	A	536	THR	5.6
1	F	211	VAL	5.6
1	L	229	ASN	5.6
1	H	88	VAL	5.6
1	B	409	CYS	5.6
1	G	222	LEU	5.6
1	B	141	PRO	5.6
1	H	318	ALA	5.6
1	L	329	GLY	5.6
1	G	343	SER	5.6
1	H	396	MET	5.6
1	G	112	VAL	5.5
1	F	186	ALA	5.5
1	H	238	PHE	5.5
1	I	550	SER	5.5
1	A	406	VAL	5.5
1	C	579	VAL	5.5
1	B	270	TYR	5.5
1	H	232	LYS	5.5
1	L	198	LEU	5.5
1	F	447	ALA	5.5
1	H	313	ALA	5.5
1	H	223	THR	5.5
1	K	282	GLU	5.5
1	A	219	LEU	5.5
1	H	317	LEU	5.5
1	F	581	TRP	5.5
1	H	602	ASN	5.5
1	L	150	ASP	5.5
1	H	390	GLY	5.5
1	K	100	PRO	5.5
1	L	195	VAL	5.5
1	F	254	SER	5.5

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Mol	Chain	Res	Type	RSRZ
1	A	214	LEU	5.5
1	B	385	LEU	5.5
1	A	583	PHE	5.5
1	H	156	PHE	5.5
1	B	322	ASN	5.5
1	G	392	MET	5.5
1	H	192	CYS	5.5
1	G	141	PRO	5.5
1	A	207	VAL	5.5
1	D	195	VAL	5.5
1	E	330	VAL	5.5
1	H	405	ALA	5.5
1	A	541	TYR	5.5
1	G	243	PHE	5.5
1	A	375	GLY	5.5
1	I	363	GLY	5.5
1	I	204	LYS	5.5
1	A	593	VAL	5.5
1	E	421	VAL	5.5
1	F	230	VAL	5.5
1	K	148	VAL	5.5
1	G	385	LEU	5.5
1	H	196	ALA	5.5
1	J	297	LEU	5.5
1	C	462	GLY	5.4
1	H	228	ILE	5.4
1	I	264	ILE	5.4
1	B	258	ASN	5.4
1	E	137	LYS	5.4
1	L	157	LEU	5.4
1	I	477	GLY	5.4
1	C	275	ASP	5.4
1	J	388	ALA	5.4
1	K	128	THR	5.4
1	I	162	MET	5.4
1	I	364	ASP	5.4
1	E	510	ILE	5.4
1	C	581	TRP	5.4
1	G	577	ALA	5.4
1	H	364	ASP	5.4
1	L	298	ILE	5.4
1	G	462	GLY	5.4

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Mol	Chain	Res	Type	RSRZ
1	C	385	LEU	5.4
1	F	297	LEU	5.4
1	G	487	LEU	5.4
1	H	336	LEU	5.4
1	I	153	VAL	5.4
1	J	315	VAL	5.4
1	D	149	ASN	5.4
1	A	544	ILE	5.4
1	G	393	ILE	5.4
1	H	110	ILE	5.4
1	H	485	ALA	5.4
1	J	114	VAL	5.4
1	K	195	VAL	5.4
1	A	391	SER	5.4
1	H	273	ASN	5.4
1	J	164	LYS	5.4
1	L	237	PHE	5.4
1	H	205	ARG	5.4
1	L	162	MET	5.4
1	E	117	ILE	5.3
1	G	144	ILE	5.3
1	A	154	SER	5.3
1	G	214	LEU	5.3
1	L	219	LEU	5.3
1	L	583	PHE	5.3
1	I	261	MET	5.3
1	C	393	ILE	5.3
1	D	412	CYS	5.3
1	E	445	ILE	5.3
1	I	274	ALA	5.3
1	B	330	VAL	5.3
1	F	323	LEU	5.3
1	H	167	VAL	5.3
1	I	308	VAL	5.3
1	J	595	LEU	5.3
1	L	470	LEU	5.3
1	L	398	PHE	5.3
1	E	277	TYR	5.3
1	B	340	ALA	5.3
1	A	537	LEU	5.3
1	C	601	LEU	5.3
1	F	198	LEU	5.3

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Mol	Chain	Res	Type	RSRZ
1	F	187	VAL	5.3
1	J	335	GLU	5.3
1	I	134	ASN	5.3
1	H	472	TYR	5.3
1	D	395	LEU	5.3
1	H	259	VAL	5.3
1	H	478	VAL	5.3
1	G	582	ASN	5.3
1	I	238	PHE	5.3
1	H	302	SER	5.3
1	A	298	ILE	5.3
1	G	389	PRO	5.3
1	I	310	LEU	5.3
1	C	192	CYS	5.3
1	F	493	TYR	5.3
1	H	181	ASN	5.3
1	K	495	LEU	5.3
1	A	365	VAL	5.2
1	E	429	VAL	5.2
1	K	153	VAL	5.2
1	D	369	ILE	5.2
1	E	446	THR	5.2
1	A	581	TRP	5.2
1	C	183	ASN	5.2
1	E	229	ASN	5.2
1	I	133	ASN	5.2
1	J	122	ASN	5.2
1	I	287	TYR	5.2
1	A	426	LEU	5.2
1	D	94	LEU	5.2
1	I	595	LEU	5.2
1	A	87	GLU	5.2
1	C	400	MET	5.2
1	F	491	MET	5.2
1	C	565	PHE	5.2
1	G	119	GLY	5.2
1	H	233	ASN	5.2
1	E	99	ILE	5.2
1	G	526	TRP	5.2
1	H	198	LEU	5.2
1	J	426	LEU	5.2
1	A	551	VAL	5.2

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Mol	Chain	Res	Type	RSRZ
1	L	577	ALA	5.2
1	D	363	GLY	5.2
1	E	106	PRO	5.2
1	H	203	MET	5.2
1	E	237	PHE	5.2
1	I	377	THR	5.2
1	A	107	ILE	5.2
1	A	271	ILE	5.2
1	J	279	GLU	5.2
1	K	297	LEU	5.2
1	I	209	SER	5.2
1	D	551	VAL	5.2
1	E	281	VAL	5.2
1	K	420	ASN	5.2
1	A	274	ALA	5.2
1	H	140	GLY	5.2
1	K	405	ALA	5.2
1	J	261	MET	5.2
1	J	280	GLU	5.2
1	J	488	THR	5.2
1	I	271	ILE	5.2
1	F	146	SER	5.2
1	G	480	TYR	5.2
1	A	104[A]	ASN	5.2
1	G	229	ASN	5.2
1	F	286	VAL	5.2
1	I	114	VAL	5.2
1	L	340	ALA	5.2
1	G	275	ASP	5.2
1	C	423	ILE	5.2
1	A	511	ASN	5.2
1	F	273	ASN	5.2
1	G	239	LEU	5.2
1	G	596	LEU	5.2
1	I	566	VAL	5.2
1	K	191	GLY	5.2
1	L	126	GLY	5.2
1	L	140	GLY	5.2
1	A	109	ASP	5.2
1	C	141	PRO	5.2
1	K	490	ALA	5.2
1	H	226	PHE	5.1

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Mol	Chain	Res	Type	RSRZ
1	C	273	ASN	5.1
1	K	484	ILE	5.1
1	A	407	LEU	5.1
1	C	290	GLY	5.1
1	I	478	VAL	5.1
1	B	410	ALA	5.1
1	D	138	GLU	5.1
1	D	261	MET	5.1
1	H	199	SER	5.1
1	G	107	ILE	5.1
1	I	107	ILE	5.1
1	B	364	ASP	5.1
1	C	256	ASP	5.1
1	I	333	LEU	5.1
1	A	206	VAL	5.1
1	B	259	VAL	5.1
1	B	308	VAL	5.1
1	B	439	TYR	5.1
1	H	274	ALA	5.1
1	J	467	ALA	5.1
1	H	362	LYS	5.1
1	I	183	ASN	5.1
1	B	193	GLY	5.1
1	E	275	ASP	5.1
1	F	136	GLY	5.1
1	G	136	GLY	5.1
1	J	262	GLU	5.1
1	F	562	LEU	5.1
1	I	514	LEU	5.1
1	J	239	LEU	5.1
1	A	257	LYS	5.1
1	A	546	GLN	5.1
1	C	181	ASN	5.1
1	E	541	TYR	5.1
1	F	263	TYR	5.1
1	F	405	ALA	5.1
1	G	372	VAL	5.1
1	H	195	VAL	5.1
1	J	299	ALA	5.1
1	K	308	VAL	5.1
1	K	486	THR	5.1
1	L	379	ASP	5.1

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Mol	Chain	Res	Type	RSRZ
1	G	547	ILE	5.1
1	B	597	THR	5.1
1	E	406	VAL	5.1
1	G	276	THR	5.1
1	C	121	CYS	5.1
1	C	376	ILE	5.1
1	G	354	PHE	5.1
1	K	101	ILE	5.1
1	F	470	LEU	5.1
1	G	297	LEU	5.1
1	J	94	LEU	5.1
1	H	197	ASP	5.1
1	L	231	ASP	5.1
1	A	452	THR	5.1
1	L	486	THR	5.1
1	I	365	VAL	5.1
1	C	292	TYR	5.1
1	I	411	TYR	5.1
1	L	189	TYR	5.1
1	A	400	MET	5.1
1	J	121	CYS	5.1
1	G	544	ILE	5.1
1	F	328	LEU	5.0
1	G	514	LEU	5.0
1	B	318	ALA	5.0
1	G	146	SER	5.0
1	D	148	VAL	5.0
1	D	185	VAL	5.0
1	D	207	VAL	5.0
1	G	315	VAL	5.0
1	J	557	VAL	5.0
1	D	472	TYR	5.0
1	C	228	ILE	5.0
1	C	555	SER	5.0
1	F	435	SER	5.0
1	C	404	ALA	5.0
1	E	558	ALA	5.0
1	I	276	THR	5.0
1	K	340	ALA	5.0
1	B	365	VAL	5.0
1	G	434	VAL	5.0
1	G	579	VAL	5.0

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Mol	Chain	Res	Type	RSRZ
1	K	557	VAL	5.0
1	L	277	TYR	5.0
1	F	576	ILE	5.0
1	H	445	ILE	5.0
1	C	537	LEU	5.0
1	G	169	LEU	5.0
1	H	492	LEU	5.0
1	I	242	LEU	5.0
1	J	219	LEU	5.0
1	J	495	LEU	5.0
1	L	199	SER	5.0
1	C	286	VAL	5.0
1	G	135	PRO	5.0
1	F	154	SER	5.0
1	G	583	PHE	5.0
1	B	371	LEU	5.0
1	D	297	LEU	5.0
1	C	486	THR	5.0
1	E	196	ALA	5.0
1	F	488	THR	5.0
1	I	553	ALA	5.0
1	K	274	ALA	5.0
1	C	305	CYS	5.0
1	C	207	VAL	5.0
1	A	246	TYR	5.0
1	A	144	ILE	5.0
1	A	530	ILE	5.0
1	I	376	ILE	5.0
1	K	291	THR	5.0
1	L	473	ALA	5.0
1	J	430	CYS	5.0
1	G	331	LYS	5.0
1	H	153	VAL	5.0
1	K	315	VAL	5.0
1	E	349	MET	5.0
1	B	477	GLY	5.0
1	K	311	SER	5.0
1	K	549	SER	5.0
1	H	176	TYR	5.0
1	H	277	TYR	5.0
1	J	411	TYR	5.0
1	G	258	ASN	5.0

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Mol	Chain	Res	Type	RSRZ
1	L	149	ASN	5.0
1	B	393	ILE	5.0
1	A	385	LEU	5.0
1	B	105	THR	5.0
1	E	562	LEU	5.0
1	F	223	THR	5.0
1	H	385	LEU	5.0
1	L	289	PHE	5.0
1	L	465	THR	5.0
1	L	561	PHE	5.0
1	A	167	VAL	4.9
1	A	372	VAL	4.9
1	B	482	VAL	4.9
1	D	211	VAL	4.9
1	K	434	VAL	4.9
1	K	524	VAL	4.9
1	C	247	MET	4.9
1	D	549	SER	4.9
1	E	345	GLY	4.9
1	E	548	SER	4.9
1	I	580	SER	4.9
1	K	559	SER	4.9
1	I	196	ALA	4.9
1	J	574	ILE	4.9
1	I	357	LEU	4.9
1	L	210	LEU	4.9
1	L	426	LEU	4.9
1	I	262	GLU	4.9
1	J	389	PRO	4.9
1	D	187	VAL	4.9
1	H	571	TRP	4.9
1	L	123	VAL	4.9
1	L	132	VAL	4.9
1	J	349	MET	4.9
1	K	113	GLN	4.9
1	E	291	THR	4.9
1	F	304	TYR	4.9
1	G	266	HIS	4.9
1	G	402	GLY	4.9
1	H	351	PRO	4.9
1	H	511	ASN	4.9
1	K	207	VAL	4.9

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Mol	Chain	Res	Type	RSRZ
1	I	247	MET	4.9
1	C	200	GLU	4.9
1	D	409	CYS	4.9
1	G	263	TYR	4.9
1	K	115	TYR	4.9
1	A	198	LEU	4.9
1	D	178	PHE	4.9
1	K	492	LEU	4.9
1	L	321	LEU	4.9
1	F	582	ASN	4.9
1	G	145	SER	4.9
1	D	429	VAL	4.9
1	F	571	TRP	4.9
1	E	276	THR	4.9
1	F	452	THR	4.9
1	A	460	ALA	4.9
1	A	264	ILE	4.9
1	D	192	CYS	4.9
1	J	513	ILE	4.9
1	D	390	GLY	4.9
1	E	309	SER	4.9
1	J	135	PRO	4.9
1	A	197	ASP	4.9
1	G	128	THR	4.9
1	E	577	ALA	4.9
1	J	450	GLY	4.9
1	E	559	SER	4.9
1	G	244	TYR	4.9
1	K	541	TYR	4.9
1	F	156	PHE	4.9
1	F	583	PHE	4.9
1	G	588	PRO	4.9
1	J	403	CYS	4.9
1	E	507	GLU	4.9
1	F	421	VAL	4.9
1	H	116	ASP	4.9
1	B	396	MET	4.9
1	B	183	ASN	4.9
1	H	322	ASN	4.9
1	L	139	ASN	4.9
1	A	313	ALA	4.8
1	G	473	ALA	4.8

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Mol	Chain	Res	Type	RSRZ
1	H	428	ALA	4.8
1	C	257	LYS	4.8
1	A	376	ILE	4.8
1	B	333	LEU	4.8
1	C	323	LEU	4.8
1	F	219	LEU	4.8
1	H	393	ILE	4.8
1	H	484	ILE	4.8
1	H	556	ILE	4.8
1	B	599	PHE	4.8
1	G	499	TYR	4.8
1	A	112	VAL	4.8
1	A	195	VAL	4.8
1	G	123	VAL	4.8
1	K	593	VAL	4.8
1	A	486	THR	4.8
1	K	390	GLY	4.8
1	I	490	ALA	4.8
1	F	101	ILE	4.8
1	K	487	LEU	4.8
1	B	176	TYR	4.8
1	G	543	ASP	4.8
1	I	591	PHE	4.8
1	L	480	TYR	4.8
1	H	174	HIS	4.8
1	K	166	ASN	4.8
1	C	162	MET	4.8
1	D	557	VAL	4.8
1	I	392	MET	4.8
1	A	393	ILE	4.8
1	B	107	ILE	4.8
1	C	298	ILE	4.8
1	D	544	ILE	4.8
1	F	466	LEU	4.8
1	I	562	LEU	4.8
1	J	376	ILE	4.8
1	G	362	LYS	4.8
1	L	158	LYS	4.8
1	E	292	TYR	4.8
1	F	287	TYR	4.8
1	B	566	VAL	4.8
1	C	248	THR	4.8

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Mol	Chain	Res	Type	RSRZ
1	C	338	MET	4.8
1	B	180	ASP	4.8
1	E	362	LYS	4.8
1	L	552	LYS	4.8
1	K	117	ILE	4.8
1	L	333	LEU	4.8
1	L	395	LEU	4.8
1	C	229	ASN	4.8
1	A	561	PHE	4.8
1	C	165	PHE	4.8
1	F	289	PHE	4.8
1	C	550	SER	4.8
1	G	291	THR	4.8
1	C	135	PRO	4.8
1	I	100	PRO	4.8
1	I	473	ALA	4.8
1	L	387	ALA	4.8
1	D	487	LEU	4.8
1	E	210	LEU	4.8
1	E	492	LEU	4.8
1	F	242	LEU	4.8
1	A	547	ILE	4.8
1	F	373	GLY	4.8
1	G	268	GLY	4.8
1	D	439	TYR	4.8
1	C	146	SER	4.8
1	C	150	ASP	4.8
1	C	344	VAL	4.8
1	J	455	VAL	4.8
1	K	485	ALA	4.8
1	L	330	VAL	4.8
1	E	385	LEU	4.8
1	B	117	ILE	4.8
1	E	382	GLY	4.8
1	K	578	GLY	4.8
1	D	197	ASP	4.7
1	C	493	TYR	4.7
1	E	569	THR	4.7
1	B	602	ASN	4.7
1	F	161	ASN	4.7
1	H	387	ALA	4.7
1	I	201	ALA	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	286	VAL	4.7
1	B	174	HIS	4.7
1	B	207	VAL	4.7
1	I	211	VAL	4.7
1	J	579	VAL	4.7
1	L	478	VAL	4.7
1	E	487	LEU	4.7
1	F	298	ILE	4.7
1	K	547	ILE	4.7
1	L	409	CYS	4.7
1	G	115	TYR	4.7
1	I	299	ALA	4.7
1	C	557	VAL	4.7
1	F	113	GLN	4.7
1	F	281	VAL	4.7
1	F	551	VAL	4.7
1	H	551	VAL	4.7
1	F	402	GLY	4.7
1	I	275	ASP	4.7
1	B	110	ILE	4.7
1	E	355	ILE	4.7
1	F	129	ILE	4.7
1	K	348	SER	4.7
1	E	278	LYS	4.7
1	K	192	CYS	4.7
1	H	258	ASN	4.7
1	F	176	TYR	4.7
1	F	277	TYR	4.7
1	G	186	ALA	4.7
1	J	493	TYR	4.7
1	B	159	ASP	4.7
1	B	203	MET	4.7
1	D	180	ASP	4.7
1	E	373	GLY	4.7
1	G	413	VAL	4.7
1	K	190	VAL	4.7
1	G	137	LYS	4.7
1	B	323	LEU	4.7
1	L	94	LEU	4.7
1	L	242	LEU	4.7
1	L	537	LEU	4.7
1	D	233	ASN	4.7

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Mol	Chain	Res	Type	RSRZ
1	F	99	ILE	4.7
1	J	229	ASN	4.7
1	J	305	CYS	4.7
1	I	197	ASP	4.7
1	E	140	GLY	4.7
1	E	383	TYR	4.7
1	E	592	GLY	4.7
1	H	293	TYR	4.7
1	L	268	GLY	4.7
1	A	434	VAL	4.7
1	I	330	VAL	4.7
1	L	286	VAL	4.7
1	L	579	VAL	4.7
1	E	343	SER	4.7
1	L	146	SER	4.7
1	G	301	PRO	4.7
1	B	366	LYS	4.7
1	F	409	CYS	4.7
1	D	203	MET	4.7
1	A	515	GLN	4.7
1	I	524	VAL	4.7
1	J	230	VAL	4.7
1	J	478	VAL	4.7
1	K	401	SER	4.7
1	L	515	GLN	4.7
1	E	495	LEU	4.7
1	G	395	LEU	4.7
1	B	137	LYS	4.7
1	C	364	ASP	4.7
1	L	556	ILE	4.7
1	H	477	GLY	4.7
1	E	121	CYS	4.6
1	H	179	ASN	4.6
1	H	190	VAL	4.6
1	K	482	VAL	4.6
1	F	394	ASP	4.6
1	J	150	ASP	4.6
1	B	514	LEU	4.6
1	E	537	LEU	4.6
1	H	357	LEU	4.6
1	K	155	GLU	4.6
1	B	171	THR	4.6

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Mol	Chain	Res	Type	RSRZ
1	L	418	PRO	4.6
1	A	473	ALA	4.6
1	B	370	ALA	4.6
1	C	252	PHE	4.6
1	C	296	GLN	4.6
1	D	387	ALA	4.6
1	E	300	ALA	4.6
1	F	558	ALA	4.6
1	K	306	ASN	4.6
1	J	550	SER	4.6
1	E	524	VAL	4.6
1	E	593	VAL	4.6
1	G	593	VAL	4.6
1	H	227	GLU	4.6
1	F	596	LEU	4.6
1	H	371	LEU	4.6
1	A	496	GLY	4.6
1	B	513	ILE	4.6
1	K	393	ILE	4.6
1	E	581	TRP	4.6
1	H	585	ALA	4.6
1	J	599	PHE	4.6
1	K	398	PHE	4.6
1	C	197	ASP	4.6
1	I	150	ASP	4.6
1	K	184	SER	4.6
1	F	177	MET	4.6
1	E	493	TYR	4.6
1	H	429	VAL	4.6
1	A	342	LEU	4.6
1	B	267	LEU	4.6
1	B	464	LEU	4.6
1	D	470	LEU	4.6
1	H	219	LEU	4.6
1	L	276	THR	4.6
1	L	444	ILE	4.6
1	D	294	ALA	4.6
1	G	387	ALA	4.6
1	K	175	PHE	4.6
1	K	550	SER	4.6
1	B	331	LYS	4.6
1	B	433	MET	4.6

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Mol	Chain	Res	Type	RSRZ
1	I	396	MET	4.6
1	B	472	TYR	4.6
1	C	381	GLY	4.6
1	G	592	GLY	4.6
1	H	206	VAL	4.6
1	J	551	VAL	4.6
1	L	120	GLY	4.6
1	C	258	ASN	4.6
1	D	273	ASN	4.6
1	F	395	LEU	4.6
1	G	127	LEU	4.6
1	G	323	LEU	4.6
1	I	171	THR	4.6
1	K	407	LEU	4.6
1	A	430	CYS	4.6
1	B	116	ASP	4.6
1	H	271	ILE	4.6
1	L	529	ILE	4.6
1	C	405	ALA	4.6
1	I	145	SER	4.6
1	H	398	PHE	4.6
1	H	565	PHE	4.6
1	J	552	LYS	4.6
1	B	280	GLU	4.6
1	A	330	VAL	4.6
1	E	112	VAL	4.6
1	I	92	VAL	4.6
1	L	528	PRO	4.6
1	L	551	VAL	4.6
1	G	256	ASP	4.6
1	B	395	LEU	4.6
1	G	219	LEU	4.6
1	H	242	LEU	4.6
1	J	466	LEU	4.6
1	L	342	LEU	4.6
1	L	488	THR	4.6
1	A	584	LYS	4.6
1	D	401	SER	4.6
1	J	517	SER	4.6
1	K	417	LYS	4.6
1	L	107	ILE	4.6
1	F	485	ALA	4.6

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Mol	Chain	Res	Type	RSRZ
1	L	460	ALA	4.6
1	A	134	ASN	4.6
1	A	329	GLY	4.6
1	A	392	MET	4.6
1	B	179	ASN	4.6
1	F	432	ASN	4.6
1	H	462	GLY	4.6
1	K	441	PRO	4.6
1	C	276	THR	4.6
1	D	137	LYS	4.6
1	I	148	VAL	4.6
1	A	287	TYR	4.6
1	B	263	TYR	4.6
1	C	466	LEU	4.6
1	G	464	LEU	4.6
1	H	466	LEU	4.6
1	L	466	LEU	4.6
1	E	520	SER	4.5
1	D	484	ILE	4.5
1	H	473	ALA	4.5
1	I	300	ALA	4.5
1	J	410	ALA	4.5
1	A	403	CYS	4.5
1	K	409	CYS	4.5
1	A	180	ASP	4.5
1	F	119	GLY	4.5
1	G	382	GLY	4.5
1	L	565	PHE	4.5
1	C	143	LYS	4.5
1	L	182	LYS	4.5
1	K	392	MET	4.5
1	D	524	VAL	4.5
1	I	344	VAL	4.5
1	A	560	LEU	4.5
1	A	453	ILE	4.5
1	E	453	ILE	4.5
1	B	164	LYS	4.5
1	E	306	ASN	4.5
1	F	134	ASN	4.5
1	E	504	GLY	4.5
1	F	362	LYS	4.5
1	H	147	LYS	4.5

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Mol	Chain	Res	Type	RSRZ
1	H	538	ASN	4.5
1	D	378	PHE	4.5
1	H	403	CYS	4.5
1	E	295	SER	4.5
1	L	455	VAL	4.5
1	L	600	VAL	4.5
1	A	439	TYR	4.5
1	J	405	ALA	4.5
1	G	381	GLY	4.5
1	A	389	PRO	4.5
1	C	583	PHE	4.5
1	E	398	PHE	4.5
1	G	565	PHE	4.5
1	I	252	PHE	4.5
1	K	220	SER	4.5
1	C	394	ASP	4.5
1	C	434	VAL	4.5
1	C	502	VAL	4.5
1	F	507	GLU	4.5
1	G	357	LEU	4.5
1	I	434	VAL	4.5
1	L	116	ASP	4.5
1	L	207	VAL	4.5
1	A	115	TYR	4.5
1	A	383	TYR	4.5
1	B	462	GLY	4.5
1	F	347	GLY	4.5
1	L	383	TYR	4.5
1	C	510	ILE	4.5
1	D	223	THR	4.5
1	D	486	THR	4.5
1	H	162	MET	4.5
1	J	400	MET	4.5
1	G	260	ASN	4.5
1	G	121	CYS	4.5
1	C	514	LEU	4.5
1	E	230	VAL	4.5
1	I	88	VAL	4.5
1	I	537	LEU	4.5
1	L	187	VAL	4.5
1	B	300	ALA	4.5
1	D	467	ALA	4.5

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Mol	Chain	Res	Type	RSRZ
1	G	201	ALA	4.5
1	L	294	ALA	4.5
1	A	111	LYS	4.5
1	A	445	ILE	4.5
1	D	228	ILE	4.5
1	D	376	ILE	4.5
1	B	457	ASN	4.5
1	C	322	ASN	4.5
1	F	486	THR	4.5
1	K	602	ASN	4.5
1	L	241	THR	4.5
1	H	131	LEU	4.5
1	I	198	LEU	4.5
1	L	451	LYS	4.5
1	C	410	ALA	4.5
1	C	542	ALA	4.5
1	F	404	ALA	4.5
1	H	340	ALA	4.5
1	J	542	ALA	4.5
1	A	574	ILE	4.5
1	H	439	TYR	4.5
1	B	217	ASN	4.4
1	B	565	PHE	4.4
1	C	261	MET	4.4
1	D	552	LYS	4.4
1	E	486	THR	4.4
1	G	561	PHE	4.4
1	G	396	MET	4.4
1	G	589	LYS	4.4
1	A	382	GLY	4.4
1	C	450	GLY	4.4
1	A	211	VAL	4.4
1	C	148	VAL	4.4
1	D	210	LEU	4.4
1	D	495	LEU	4.4
1	F	372	VAL	4.4
1	G	310	LEU	4.4
1	H	297	LEU	4.4
1	I	234	LEU	4.4
1	K	298	ILE	4.4
1	E	115	TYR	4.4
1	B	362	LYS	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	398	PHE	4.4
1	E	425	PHE	4.4
1	I	130	PHE	4.4
1	K	488	THR	4.4
1	H	177	MET	4.4
1	K	396	MET	4.4
1	A	314	ALA	4.4
1	A	387	ALA	4.4
1	G	195	VAL	4.4
1	G	447	ALA	4.4
1	H	479	ASP	4.4
1	I	372	VAL	4.4
1	K	579	VAL	4.4
1	L	558	ALA	4.4
1	H	111	LYS	4.4
1	A	133	ASN	4.4
1	H	133	ASN	4.4
1	B	298	ILE	4.4
1	L	453	ILE	4.4
1	A	176	TYR	4.4
1	J	412	CYS	4.4
1	E	354	PHE	4.4
1	K	583	PHE	4.4
1	C	543	ASP	4.4
1	F	118	LYS	4.4
1	G	111	LYS	4.4
1	A	467	ALA	4.4
1	A	553	ALA	4.4
1	C	387	ALA	4.4
1	E	404	ALA	4.4
1	F	321	LEU	4.4
1	F	585	ALA	4.4
1	G	407	LEU	4.4
1	H	169	LEU	4.4
1	A	224	VAL	4.4
1	I	421	VAL	4.4
1	G	295	SER	4.4
1	K	363	GLY	4.4
1	G	248	THR	4.4
1	F	237	PHE	4.4
1	A	229	ASN	4.4
1	K	313	ALA	4.4

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Mol	Chain	Res	Type	RSRZ
1	C	464	LEU	4.4
1	D	302	SER	4.4
1	G	142	VAL	4.4
1	J	348	SER	4.4
1	B	504	GLY	4.4
1	C	99	ILE	4.4
1	H	337	LYS	4.4
1	J	99	ILE	4.4
1	J	138	GLU	4.4
1	A	480	TYR	4.4
1	C	541	TYR	4.4
1	D	244	TYR	4.4
1	I	103	TYR	4.4
1	L	341	TYR	4.4
1	C	294	ALA	4.4
1	E	528	PRO	4.4
1	H	301	PRO	4.4
1	H	410	ALA	4.4
1	K	307	PRO	4.4
1	A	127	LEU	4.4
1	D	86	SER	4.4
1	E	560	LEU	4.4
1	H	524	VAL	4.4
1	L	344	VAL	4.4
1	I	329	GLY	4.4
1	G	129	ILE	4.4
1	G	171	THR	4.4
1	G	285	ARG	4.4
1	D	457	ASN	4.4
1	E	565	PHE	4.4
1	G	552	LYS	4.4
1	H	247	MET	4.4
1	I	589	LYS	4.4
1	K	518	LYS	4.4
1	A	412	CYS	4.4
1	C	577	ALA	4.4
1	E	550	SER	4.4
1	F	553	ALA	4.4
1	J	549	SER	4.4
1	L	313	ALA	4.4
1	A	456	GLY	4.3
1	A	464	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
1	H	214	LEU	4.3
1	B	114	VAL	4.3
1	B	372	VAL	4.3
1	I	406	VAL	4.3
1	J	88	VAL	4.3
1	L	372	VAL	4.3
1	A	423	ILE	4.3
1	G	110	ILE	4.3
1	H	161	ASN	4.3
1	I	582	ASN	4.3
1	J	556	ILE	4.3
1	I	288	TYR	4.3
1	A	599	PHE	4.3
1	I	526	TRP	4.3
1	B	140	GLY	4.3
1	F	462	GLY	4.3
1	G	120	GLY	4.3
1	K	339	GLY	4.3
1	A	466	LEU	4.3
1	A	470	LEU	4.3
1	H	395	LEU	4.3
1	C	185	VAL	4.3
1	J	185	VAL	4.3
1	L	224	VAL	4.3
1	A	137	LYS	4.3
1	B	479	ASP	4.3
1	G	162	MET	4.3
1	H	440	ARG	4.3
1	I	115	TYR	4.3
1	B	178	PHE	4.3
1	D	318	ALA	4.3
1	D	599	PHE	4.3
1	G	469	ALA	4.3
1	J	85	ALA	4.3
1	J	331	LYS	4.3
1	J	272	ASN	4.3
1	A	308	VAL	4.3
1	B	248	THR	4.3
1	G	264	ILE	4.3
1	G	484	ILE	4.3
1	A	361	SER	4.3
1	A	469	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	177	MET	4.3
1	F	499	TYR	4.3
1	G	176	TYR	4.3
1	L	533	TYR	4.3
1	K	432	ASN	4.3
1	A	239	LEU	4.3
1	I	426	LEU	4.3
1	I	560	LEU	4.3
1	F	315	VAL	4.3
1	F	557	VAL	4.3
1	L	365	VAL	4.3
1	C	97	THR	4.3
1	I	465	THR	4.3
1	G	298	ILE	4.3
1	H	510	ILE	4.3
1	L	164	LYS	4.3
1	L	484	ILE	4.3
1	C	140	GLY	4.3
1	E	119	GLY	4.3
1	D	405	ALA	4.3
1	L	270	TYR	4.3
1	E	464	LEU	4.3
1	H	310	LEU	4.3
1	I	317	LEU	4.3
1	J	596	LEU	4.3
1	L	127	LEU	4.3
1	D	147	LYS	4.3
1	F	593	VAL	4.3
1	G	180	ASP	4.3
1	I	281	VAL	4.3
1	K	206	VAL	4.3
1	L	225	VAL	4.3
1	E	298	ILE	4.3
1	E	401	SER	4.3
1	K	295	SER	4.3
1	A	390	GLY	4.3
1	F	120	GLY	4.3
1	G	412	CYS	4.3
1	J	192	CYS	4.3
1	K	408	GLY	4.3
1	A	531	ASN	4.3
1	E	312	ASN	4.3

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Mol	Chain	Res	Type	RSRZ
1	K	217	ASN	4.3
1	G	558	ALA	4.3
1	D	541	TYR	4.3
1	F	115	TYR	4.3
1	G	197	ASP	4.3
1	C	119	GLY	4.3
1	B	511	ASN	4.2
1	C	420	ASN	4.2
1	D	449	ASN	4.2
1	F	529	ILE	4.2
1	J	529	ILE	4.2
1	D	279	GLU	4.2
1	L	274	ALA	4.2
1	C	392	MET	4.2
1	B	297	LEU	4.2
1	C	495	LEU	4.2
1	E	94	LEU	4.2
1	E	472	TYR	4.2
1	H	560	LEU	4.2
1	L	214	LEU	4.2
1	L	371	LEU	4.2
1	C	494	SER	4.2
1	D	391	SER	4.2
1	H	184	SER	4.2
1	K	188	GLY	4.2
1	A	225	VAL	4.2
1	C	308	VAL	4.2
1	E	478	VAL	4.2
1	H	112	VAL	4.2
1	J	260	ASN	4.2
1	B	108	HIS	4.2
1	B	369	ILE	4.2
1	G	376	ILE	4.2
1	L	576	ILE	4.2
1	K	202	ASP	4.2
1	L	490	ALA	4.2
1	D	561	PHE	4.2
1	A	234	LEU	4.2
1	C	94	LEU	4.2
1	C	411	TYR	4.2
1	D	560	LEU	4.2
1	K	122	ASN	4.2

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Mol	Chain	Res	Type	RSRZ
1	K	302	SER	4.2
1	L	169	LEU	4.2
1	E	329	GLY	4.2
1	H	139	ASN	4.2
1	K	597	THR	4.2
1	K	96	PRO	4.2
1	K	224	VAL	4.2
1	I	180	ASP	4.2
1	L	355	ILE	4.2
1	C	313	ALA	4.2
1	D	490	ALA	4.2
1	A	203	MET	4.2
1	A	145	SER	4.2
1	B	302	SER	4.2
1	B	412	CYS	4.2
1	C	295	SER	4.2
1	D	448	SER	4.2
1	G	154	SER	4.2
1	G	175	PHE	4.2
1	H	152	GLN	4.2
1	H	305	CYS	4.2
1	H	425	PHE	4.2
1	J	104	ASN	4.2
1	J	384	ASN	4.2
1	J	390	GLY	4.2
1	K	503	PHE	4.2
1	D	492	LEU	4.2
1	I	601	LEU	4.2
1	L	495	LEU	4.2
1	D	493	TYR	4.2
1	H	263	TYR	4.2
1	I	472	TYR	4.2
1	B	211	VAL	4.2
1	J	112	VAL	4.2
1	L	206	VAL	4.2
1	B	158	LYS	4.2
1	E	393	ILE	4.2
1	B	405	ALA	4.2
1	K	581	TRP	4.2
1	D	442	GLY	4.2
1	J	392	MET	4.2
1	E	172	SER	4.2

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Mol	Chain	Res	Type	RSRZ
1	J	145	SER	4.2
1	L	391	SER	4.2
1	A	297	LEU	4.2
1	A	378	PHE	4.2
1	H	127	LEU	4.2
1	I	165	PHE	4.2
1	I	371	LEU	4.2
1	K	275	ASP	4.2
1	L	394	ASP	4.2
1	L	459	ASP	4.2
1	H	383	TYR	4.2
1	E	365	VAL	4.2
1	H	421	VAL	4.2
1	I	502	VAL	4.2
1	J	413	VAL	4.2
1	B	101	ILE	4.2
1	F	314	ALA	4.2
1	K	299	ALA	4.2
1	L	445	ILE	4.2
1	E	521	ASN	4.2
1	I	258	ASN	4.2
1	B	559	SER	4.2
1	G	580	SER	4.2
1	H	433	MET	4.2
1	I	379	ASP	4.2
1	F	426	LEU	4.2
1	K	596	LEU	4.2
1	L	130	PHE	4.2
1	F	190	VAL	4.2
1	H	281	VAL	4.2
1	C	122	ASN	4.2
1	L	545	ASN	4.2
1	A	299	ALA	4.2
1	A	558	ALA	4.2
1	C	428	ALA	4.2
1	E	513	ILE	4.2
1	E	556	ILE	4.2
1	I	484	ILE	4.2
1	C	311	SER	4.2
1	C	584	LYS	4.2
1	D	209	SER	4.2
1	E	311	SER	4.2

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Mol	Chain	Res	Type	RSRZ
1	G	138	GLU	4.2
1	G	254	SER	4.2
1	H	584	LYS	4.2
1	A	396	MET	4.1
1	L	526	TRP	4.1
1	E	595	LEU	4.1
1	H	537	LEU	4.1
1	K	426	LEU	4.1
1	B	411	TYR	4.1
1	E	272	ASN	4.1
1	G	257	LYS	4.1
1	G	421	VAL	4.1
1	I	593	VAL	4.1
1	L	566	VAL	4.1
1	J	101	ILE	4.1
1	A	162	MET	4.1
1	A	248	THR	4.1
1	H	465	THR	4.1
1	A	210	LEU	4.1
1	B	378	PHE	4.1
1	B	595	LEU	4.1
1	I	487	LEU	4.1
1	I	495	LEU	4.1
1	A	602	ASN	4.1
1	K	352	ASN	4.1
1	A	592	GLY	4.1
1	E	92	VAL	4.1
1	F	344	VAL	4.1
1	H	191	GLY	4.1
1	I	408	GLY	4.1
1	I	557	VAL	4.1
1	J	195	VAL	4.1
1	L	112	VAL	4.1
1	A	535	ALA	4.1
1	F	542	ALA	4.1
1	J	553	ALA	4.1
1	E	544	ILE	4.1
1	G	271	ILE	4.1
1	A	377	THR	4.1
1	C	171	THR	4.1
1	D	488	THR	4.1
1	F	276	THR	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	222	LEU	4.1
1	C	426	LEU	4.1
1	H	596	LEU	4.1
1	I	94	LEU	4.1
1	J	514	LEU	4.1
1	A	591	PHE	4.1
1	D	243	PHE	4.1
1	I	581	TRP	4.1
1	K	504	GLY	4.1
1	L	592	GLY	4.1
1	A	494	SER	4.1
1	B	88	VAL	4.1
1	B	230	VAL	4.1
1	D	201	ALA	4.1
1	G	167	VAL	4.1
1	K	502	VAL	4.1
1	B	232	LYS	4.1
1	C	151	LYS	4.1
1	C	307	PRO	4.1
1	D	377	THR	4.1
1	I	441	PRO	4.1
1	L	491	MET	4.1
1	A	379	ASP	4.1
1	B	95	ASP	4.1
1	G	470	LEU	4.1
1	G	601	LEU	4.1
1	C	414	GLY	4.1
1	E	290	GLY	4.1
1	G	378	PHE	4.1
1	I	398	PHE	4.1
1	B	517	SER	4.1
1	C	417	LYS	4.1
1	D	581	TRP	4.1
1	F	93	SER	4.1
1	A	500	ALA	4.1
1	C	153	VAL	4.1
1	C	533	TYR	4.1
1	E	190	VAL	4.1
1	F	472	TYR	4.1
1	K	455	VAL	4.1
1	L	287	TYR	4.1
1	L	359	TYR	4.1

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Mol	Chain	Res	Type	RSRZ
1	L	406	VAL	4.1
1	L	421	VAL	4.1
1	L	472	TYR	4.1
1	I	547	ILE	4.1
1	B	418	PRO	4.1
1	G	134	ASN	4.1
1	H	166	ASN	4.1
1	I	179	ASN	4.1
1	K	106	PRO	4.1
1	B	465	THR	4.1
1	F	412	CYS	4.1
1	D	385	LEU	4.1
1	E	357	LEU	4.1
1	G	560	LEU	4.1
1	I	347	GLY	4.1
1	I	509	LEU	4.1
1	A	405	ALA	4.1
1	E	318	ALA	4.1
1	A	139	ASN	4.1
1	A	471	VAL	4.1
1	B	273	ASN	4.1
1	C	330	VAL	4.1
1	E	153	VAL	4.1
1	G	292	TYR	4.1
1	H	107	ILE	4.1
1	H	444	ILE	4.1
1	I	423	ILE	4.1
1	I	499	TYR	4.1
1	E	419	GLU	4.1
1	L	377	THR	4.1
1	H	347	GLY	4.1
1	A	357	LEU	4.1
1	A	401	SER	4.1
1	C	333	LEU	4.1
1	E	470	LEU	4.1
1	G	194	SER	4.1
1	B	404	ALA	4.0
1	C	457	ASN	4.0
1	G	179	ASN	4.0
1	D	419	GLU	4.0
1	G	512	LYS	4.0
1	K	324	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	195	VAL	4.0
1	G	581	TRP	4.0
1	E	359	TYR	4.0
1	G	255	THR	4.0
1	G	574	ILE	4.0
1	I	244	TYR	4.0
1	D	592	GLY	4.0
1	B	495	LEU	4.0
1	G	595	LEU	4.0
1	I	492	LEU	4.0
1	A	156	PHE	4.0
1	A	289	PHE	4.0
1	B	417	LYS	4.0
1	F	182	LYS	4.0
1	G	143	LYS	4.0
1	J	273	ASN	4.0
1	F	196	ALA	4.0
1	E	440	ARG	4.0
1	B	551	VAL	4.0
1	G	224	VAL	4.0
1	H	171	THR	4.0
1	H	536	THR	4.0
1	L	581	TRP	4.0
1	D	341	TYR	4.0
1	G	277	TYR	4.0
1	G	350	TYR	4.0
1	B	194	SER	4.0
1	B	539	SER	4.0
1	E	361	SER	4.0
1	A	272	ASN	4.0
1	D	601	LEU	4.0
1	A	503	PHE	4.0
1	B	585	ALA	4.0
1	A	148	VAL	4.0
1	A	269	VAL	4.0
1	A	339	GLY	4.0
1	C	372	VAL	4.0
1	D	434	VAL	4.0
1	F	429	VAL	4.0
1	H	207	VAL	4.0
1	I	195	VAL	4.0
1	K	119	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
1	F	465	THR	4.0
1	K	248	THR	4.0
1	K	327	ILE	4.0
1	A	263	TYR	4.0
1	B	216	ASP	4.0
1	B	391	SER	4.0
1	J	277	TYR	4.0
1	A	433	MET	4.0
1	C	352	ASN	4.0
1	K	139	ASN	4.0
1	B	321	LEU	4.0
1	C	210	LEU	4.0
1	D	208	LEU	4.0
1	E	310	LEU	4.0
1	F	527	LEU	4.0
1	H	328	LEU	4.0
1	J	492	LEU	4.0
1	C	591	PHE	4.0
1	K	289	PHE	4.0
1	H	106	PRO	4.0
1	J	523	PRO	4.0
1	A	402	GLY	4.0
1	B	381	GLY	4.0
1	C	232	LYS	4.0
1	D	123	VAL	4.0
1	D	502	VAL	4.0
1	E	412	CYS	4.0
1	G	159	ASP	4.0
1	J	86	SER	4.0
1	J	306	ASN	4.0
1	H	270	TYR	4.0
1	K	293	TYR	4.0
1	K	533	TYR	4.0
1	J	509	LEU	4.0
1	L	208	LEU	4.0
1	G	158	LYS	4.0
1	H	366	LYS	4.0
1	D	398	PHE	4.0
1	E	588	PRO	4.0
1	G	485	ALA	4.0
1	G	238	PHE	4.0
1	I	237	PHE	4.0

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Mol	Chain	Res	Type	RSRZ
1	L	503	PHE	4.0
1	A	545	ASN	4.0
1	K	344	VAL	4.0
1	B	355	ILE	4.0
1	G	409	CYS	4.0
1	J	144	ILE	4.0
1	B	316	GLU	4.0
1	A	288	TYR	4.0
1	F	162	MET	4.0
1	G	541	TYR	4.0
1	D	234	LEU	4.0
1	D	596	LEU	4.0
1	H	514	LEU	4.0
1	J	127	LEU	4.0
1	K	562	LEU	4.0
1	I	382	GLY	4.0
1	I	558	ALA	4.0
1	I	577	ALA	4.0
1	L	388	ALA	4.0
1	C	237	PHE	4.0
1	J	238	PHE	4.0
1	G	273	ASN	4.0
1	F	163	GLU	4.0
1	G	488	THR	4.0
1	H	262	GLU	4.0
1	J	105	THR	4.0
1	J	458	THR	4.0
1	L	154	SER	4.0
1	A	221	LYS	4.0
1	D	88	VAL	4.0
1	G	386	LYS	4.0
1	H	406	VAL	4.0
1	C	107	ILE	3.9
1	D	355	ILE	3.9
1	K	481	ILE	3.9
1	L	129	ILE	3.9
1	L	393	ILE	3.9
1	J	409	CYS	3.9
1	K	203	MET	3.9
1	B	115	TYR	3.9
1	J	385	LEU	3.9
1	K	468	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	314	ALA	3.9
1	D	332	GLU	3.9
1	D	447	ALA	3.9
1	B	252	PHE	3.9
1	D	565	PHE	3.9
1	E	415	THR	3.9
1	G	309	SER	3.9
1	E	123	VAL	3.9
1	B	576	ILE	3.9
1	E	369	ILE	3.9
1	J	369	ILE	3.9
1	B	394	ASP	3.9
1	H	216	ASP	3.9
1	A	290	GLY	3.9
1	F	280	GLU	3.9
1	H	463	ARG	3.9
1	I	213	MET	3.9
1	A	293	TYR	3.9
1	A	341	TYR	3.9
1	C	270	TYR	3.9
1	E	293	TYR	3.9
1	F	533	TYR	3.9
1	G	492	LEU	3.9
1	H	374	LYS	3.9
1	H	441	PRO	3.9
1	K	412	CYS	3.9
1	A	384	ASN	3.9
1	B	233	ASN	3.9
1	H	495	LEU	3.9
1	D	550	SER	3.9
1	J	361	SER	3.9
1	J	555	SER	3.9
1	I	243	PHE	3.9
1	K	519	THR	3.9
1	C	513	ILE	3.9
1	F	567	GLN	3.9
1	G	308	VAL	3.9
1	L	508	GLU	3.9
1	L	574	ILE	3.9
1	B	373	GLY	3.9
1	C	402	GLY	3.9
1	A	179	ASN	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	384	ASN	3.9
1	D	229	ASN	3.9
1	E	384	ASN	3.9
1	J	217	ASN	3.9
1	A	292	TYR	3.9
1	C	439	TYR	3.9
1	H	470	LEU	3.9
1	H	493	TYR	3.9
1	I	541	TYR	3.9
1	I	596	LEU	3.9
1	K	127	LEU	3.9
1	K	464	LEU	3.9
1	E	554	SER	3.9
1	K	237	PHE	3.9
1	K	599	PHE	3.9
1	D	150	ASP	3.9
1	D	337	LYS	3.9
1	D	443	ASP	3.9
1	E	143	LYS	3.9
1	G	483	ASP	3.9
1	E	390	GLY	3.9
1	F	167	VAL	3.9
1	G	330	VAL	3.9
1	I	206	VAL	3.9
1	K	269	VAL	3.9
1	F	233	ASN	3.9
1	F	574	ILE	3.9
1	I	101	ILE	3.9
1	B	219	LEU	3.9
1	D	548	SER	3.9
1	E	407	LEU	3.9
1	F	299	ALA	3.9
1	J	125	GLU	3.9
1	J	186	ALA	3.9
1	K	98	SER	3.9
1	K	577	ALA	3.9
1	F	232	LYS	3.9
1	H	436	LYS	3.9
1	F	116	ASP	3.9
1	I	256	ASP	3.9
1	G	252	PHE	3.9
1	H	229	ASN	3.9

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Mol	Chain	Res	Type	RSRZ
1	E	101	ILE	3.9
1	K	355	ILE	3.9
1	F	301	PRO	3.9
1	A	520	SER	3.9
1	H	182	LYS	3.9
1	B	201	ALA	3.9
1	B	299	ALA	3.9
1	E	317	LEU	3.9
1	E	500	ALA	3.9
1	F	300	ALA	3.9
1	G	234	LEU	3.9
1	G	318	ALA	3.9
1	J	572	ALA	3.9
1	K	361	SER	3.9
1	L	284	ALA	3.9
1	A	569	THR	3.9
1	B	292	TYR	3.9
1	C	246	TYR	3.9
1	F	241	THR	3.9
1	G	533	TYR	3.9
1	A	165	PHE	3.9
1	A	192	CYS	3.9
1	A	322	ASN	3.9
1	B	243	PHE	3.9
1	E	505	ASN	3.9
1	G	591	PHE	3.9
1	J	565	PHE	3.9
1	A	571	TRP	3.9
1	A	331	LYS	3.9
1	F	221	LYS	3.9
1	G	540	LYS	3.9
1	F	444	ILE	3.9
1	I	123	VAL	3.9
1	J	92	VAL	3.9
1	G	401	SER	3.9
1	I	549	SER	3.9
1	J	209	SER	3.9
1	L	311	SER	3.9
1	F	371	LEU	3.9
1	H	210	LEU	3.9
1	I	527	LEU	3.9
1	J	310	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	419	GLU	3.8
1	D	480	TYR	3.8
1	L	125	GLU	3.8
1	K	587	LYS	3.8
1	A	243	PHE	3.8
1	D	591	PHE	3.8
1	E	378	PHE	3.8
1	I	226	PHE	3.8
1	J	243	PHE	3.8
1	D	418	PRO	3.8
1	E	418	PRO	3.8
1	L	571	TRP	3.8
1	A	230	VAL	3.8
1	F	264	ILE	3.8
1	G	101	ILE	3.8
1	G	187	VAL	3.8
1	G	361	SER	3.8
1	H	172	SER	3.8
1	H	427	SER	3.8
1	L	91	VAL	3.8
1	L	295	SER	3.8
1	E	485	ALA	3.8
1	I	163	GLU	3.8
1	I	410	ALA	3.8
1	A	589	LYS	3.8
1	B	257	LYS	3.8
1	D	317	LEU	3.8
1	F	407	LEU	3.8
1	H	487	LEU	3.8
1	I	97	THR	3.8
1	I	137	LYS	3.8
1	I	303	ASN	3.8
1	K	362	LYS	3.8
1	D	339	GLY	3.8
1	D	496	GLY	3.8
1	E	442	GLY	3.8
1	F	375	GLY	3.8
1	I	304	TYR	3.8
1	D	289	PHE	3.8
1	J	354	PHE	3.8
1	K	216	ASP	3.8
1	L	235	PHE	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	108	HIS	3.8
1	G	559	SER	3.8
1	H	93	SER	3.8
1	H	335	GLU	3.8
1	D	92	VAL	3.8
1	H	148	VAL	3.8
1	I	286	VAL	3.8
1	J	593	VAL	3.8
1	K	137	LYS	3.8
1	L	403	CYS	3.8
1	A	196	ALA	3.8
1	F	139	ASN	3.8
1	I	485	ALA	3.8
1	J	352	ASN	3.8
1	B	426	LEU	3.8
1	C	492	LEU	3.8
1	D	466	LEU	3.8
1	I	501	GLY	3.8
1	J	208	LEU	3.8
1	J	234	LEU	3.8
1	K	381	GLY	3.8
1	L	597	THR	3.8
1	D	270	TYR	3.8
1	J	439	TYR	3.8
1	A	254	SER	3.8
1	F	550	SER	3.8
1	H	599	PHE	3.8
1	J	254	SER	3.8
1	K	591	PHE	3.8
1	A	123	VAL	3.8
1	E	511	ASN	3.8
1	G	444	ILE	3.8
1	J	271	ILE	3.8
1	K	264	ILE	3.8
1	E	375	GLY	3.8
1	G	294	ALA	3.8
1	G	525	TRP	3.8
1	I	500	ALA	3.8
1	J	558	ALA	3.8
1	F	597	THR	3.8
1	G	198	LEU	3.8
1	H	321	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	H	446	THR	3.8
1	L	536	THR	3.8
1	D	202	ASP	3.8
1	K	150	ASP	3.8
1	I	143	LYS	3.8
1	A	472	TYR	3.8
1	C	348	SER	3.8
1	E	304	TYR	3.8
1	F	356	HIS	3.8
1	I	270	TYR	3.8
1	L	520	SER	3.8
1	H	252	PHE	3.8
1	D	352	ASN	3.8
1	F	352	ASN	3.8
1	G	139	ASN	3.8
1	G	602	ASN	3.8
1	F	594	ARG	3.8
1	A	579	VAL	3.8
1	B	313	ALA	3.8
1	C	422	GLU	3.8
1	D	315	VAL	3.8
1	D	574	ILE	3.8
1	E	574	ILE	3.8
1	H	547	ILE	3.8
1	K	138	GLU	3.8
1	K	163	GLU	3.8
1	L	471	VAL	3.8
1	L	535	ALA	3.8
1	D	433	MET	3.8
1	A	563	LYS	3.8
1	E	488	THR	3.8
1	I	283	LYS	3.8
1	I	452	THR	3.8
1	D	321	LEU	3.8
1	J	395	LEU	3.8
1	A	100	PRO	3.8
1	A	523	PRO	3.8
1	C	166	ASN	3.8
1	C	244	TYR	3.8
1	C	260	ASN	3.8
1	C	293	TYR	3.8
1	G	449	ASN	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	556	ILE	3.8
1	B	142	VAL	3.8
1	B	225	VAL	3.8
1	C	314	ALA	3.8
1	C	547	ILE	3.8
1	C	556	ILE	3.8
1	G	406	VAL	3.8
1	H	308	VAL	3.8
1	C	415	THR	3.8
1	D	248	THR	3.8
1	C	234	LEU	3.8
1	G	426	LEU	3.8
1	H	267	LEU	3.8
1	J	328	LEU	3.8
1	A	215	HIS	3.8
1	E	273	ASN	3.8
1	G	87	GLU	3.8
1	I	412	CYS	3.8
1	I	494	SER	3.8
1	K	457	ASN	3.8
1	A	118	LYS	3.8
1	A	346	LYS	3.8
1	B	552	LYS	3.8
1	C	118	LYS	3.8
1	G	118	LYS	3.8
1	A	350	TYR	3.8
1	C	408	GLY	3.7
1	H	249	ASP	3.7
1	J	381	GLY	3.7
1	J	394	ASP	3.7
1	F	274	ALA	3.7
1	A	91	VAL	3.7
1	B	291	THR	3.7
1	D	556	ILE	3.7
1	F	291	THR	3.7
1	I	212	THR	3.7
1	K	465	THR	3.7
1	K	530	ILE	3.7
1	A	285	ARG	3.7
1	C	586	ARG	3.7
1	D	200	GLU	3.7
1	G	522	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	222	LEU	3.7
1	F	127	LEU	3.7
1	F	169	LEU	3.7
1	F	464	LEU	3.7
1	G	416	LEU	3.7
1	I	208	LEU	3.7
1	B	538	ASN	3.7
1	C	199	SER	3.7
1	C	95	ASP	3.7
1	F	430	CYS	3.7
1	I	403	CYS	3.7
1	L	382	GLY	3.7
1	E	287	TYR	3.7
1	G	425	PHE	3.7
1	I	277	TYR	3.7
1	I	378	PHE	3.7
1	L	378	PHE	3.7
1	C	196	ALA	3.7
1	A	276	THR	3.7
1	A	429	VAL	3.7
1	A	484	ILE	3.7
1	C	142	VAL	3.7
1	C	167	VAL	3.7
1	C	315	VAL	3.7
1	E	195	VAL	3.7
1	D	134	ASN	3.7
1	D	396	MET	3.7
1	E	557	VAL	3.7
1	F	158	LYS	3.7
1	F	396	MET	3.7
1	K	230	VAL	3.7
1	L	557	VAL	3.7
1	H	104	ASN	3.7
1	D	438	SER	3.7
1	F	537	LEU	3.7
1	L	100	PRO	3.7
1	J	231	ASP	3.7
1	B	581	TRP	3.7
1	G	193	GLY	3.7
1	J	120	GLY	3.7
1	H	522	GLU	3.7
1	A	409	CYS	3.7

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Mol	Chain	Res	Type	RSRZ
1	G	594	ARG	3.7
1	A	103	TYR	3.7
1	A	587	LYS	3.7
1	B	189	TYR	3.7
1	C	383	TYR	3.7
1	E	367	LYS	3.7
1	E	584	LYS	3.7
1	H	103	TYR	3.7
1	H	113	GLN	3.7
1	F	340	ALA	3.7
1	H	292	TYR	3.7
1	J	270	TYR	3.7
1	B	519	THR	3.7
1	D	104	ASN	3.7
1	A	369	ILE	3.7
1	B	311	SER	3.7
1	C	361	SER	3.7
1	C	429	VAL	3.7
1	F	330	VAL	3.7
1	I	132	VAL	3.7
1	I	349	MET	3.7
1	J	498	SER	3.7
1	D	523	PRO	3.7
1	G	528	PRO	3.7
1	K	208	LEU	3.7
1	K	301	PRO	3.7
1	F	316	GLU	3.7
1	J	126	GLY	3.7
1	A	235	PHE	3.7
1	D	432	ASN	3.7
1	G	599	PHE	3.7
1	J	165	PHE	3.7
1	L	425	PHE	3.7
1	C	597	THR	3.7
1	J	244	TYR	3.7
1	L	128	THR	3.7
1	L	519	THR	3.7
1	E	231	ASP	3.7
1	E	427	SER	3.7
1	H	101	ILE	3.7
1	H	361	SER	3.7
1	K	554	SER	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	471	VAL	3.7
1	D	91	VAL	3.7
1	L	101	ILE	3.7
1	C	588	PRO	3.7
1	J	301	PRO	3.7
1	C	219	LEU	3.7
1	C	587	LYS	3.7
1	F	595	LEU	3.7
1	J	470	LEU	3.7
1	L	297	LEU	3.7
1	L	601	LEU	3.7
1	C	149	ASN	3.7
1	F	602	ASN	3.7
1	I	384	ASN	3.7
1	I	420	ASN	3.7
1	K	312	ASN	3.7
1	A	200	GLU	3.7
1	J	419	GLU	3.7
1	E	394	ASP	3.7
1	G	249	ASP	3.7
1	H	443	ASP	3.7
1	H	561	PHE	3.7
1	K	378	PHE	3.7
1	K	572	ALA	3.7
1	C	488	THR	3.7
1	C	288	TYR	3.7
1	E	480	TYR	3.7
1	C	501	GLY	3.7
1	D	445	ILE	3.7
1	E	344	VAL	3.7
1	K	373	GLY	3.7
1	E	208	LEU	3.7
1	H	562	LEU	3.7
1	K	157	LEU	3.7
1	K	310	LEU	3.7
1	L	131	LEU	3.7
1	F	306	ASN	3.7
1	C	202	ASP	3.7
1	C	137	LYS	3.7
1	F	201	ALA	3.7
1	F	266	HIS	3.7
1	I	318	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	I	573	HIS	3.7
1	A	458	THR	3.7
1	C	255	THR	3.7
1	C	354	PHE	3.7
1	C	536	THR	3.7
1	I	497	THR	3.7
1	J	378	PHE	3.7
1	B	515	GLN	3.7
1	C	523	PRO	3.7
1	E	546	GLN	3.7
1	G	375	GLY	3.7
1	I	293	TYR	3.7
1	B	187	VAL	3.7
1	C	355	ILE	3.7
1	D	393	ILE	3.7
1	F	271	ILE	3.7
1	F	508	GLU	3.6
1	F	524	VAL	3.7
1	G	269	VAL	3.7
1	H	455	VAL	3.7
1	L	315	VAL	3.7
1	L	502	VAL	3.7
1	G	94	LEU	3.6
1	J	267	LEU	3.6
1	G	133	ASN	3.6
1	A	266	HIS	3.6
1	A	348	SER	3.6
1	B	424	HIS	3.6
1	A	577	ALA	3.6
1	D	186	ALA	3.6
1	F	559	SER	3.6
1	H	550	SER	3.6
1	G	415	THR	3.6
1	J	377	THR	3.6
1	L	370	ALA	3.6
1	F	160	GLU	3.6
1	F	561	PHE	3.6
1	H	378	PHE	3.6
1	I	316	GLU	3.6
1	J	591	PHE	3.6
1	L	591	PHE	3.6
1	A	524	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	574	ILE	3.6
1	D	162	MET	3.6
1	H	99	ILE	3.6
1	H	173	LYS	3.6
1	H	264	ILE	3.6
1	H	331	LYS	3.6
1	I	99	ILE	3.6
1	I	530	ILE	3.6
1	L	493	TYR	3.6
1	E	234	LEU	3.6
1	H	200	GLU	3.6
1	E	497	THR	3.6
1	G	597	THR	3.6
1	H	469	ALA	3.6
1	I	388	ALA	3.6
1	J	428	ALA	3.6
1	K	388	ALA	3.6
1	F	100	PRO	3.6
1	B	289	PHE	3.6
1	E	217	ASN	3.6
1	E	491	MET	3.6
1	H	341	TYR	3.6
1	I	263	TYR	3.6
1	I	413	VAL	3.6
1	L	115	TYR	3.6
1	D	267	LEU	3.6
1	E	426	LEU	3.6
1	I	328	LEU	3.6
1	B	262	GLU	3.6
1	C	419	GLU	3.6
1	A	220	SER	3.6
1	D	554	SER	3.6
1	I	305	CYS	3.6
1	I	430	CYS	3.6
1	J	380	SER	3.6
1	F	589	LYS	3.6
1	A	490	ALA	3.6
1	I	255	THR	3.6
1	I	460	ALA	3.6
1	K	170	GLY	3.6
1	B	458	THR	3.6
1	L	318	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	K	588	PRO	3.6
1	A	149	ASN	3.6
1	A	275	ASP	3.6
1	D	159	ASP	3.6
1	F	104	ASN	3.6
1	G	272	ASN	3.6
1	B	586	ARG	3.6
1	F	238	PHE	3.6
1	H	243	PHE	3.6
1	J	289	PHE	3.6
1	K	102	GLU	3.6
1	C	444	ILE	3.6
1	C	484	ILE	3.6
1	A	208	LEU	3.6
1	A	321	LEU	3.6
1	B	562	LEU	3.6
1	C	206	VAL	3.6
1	C	239	LEU	3.6
1	C	416	LEU	3.6
1	C	509	LEU	3.6
1	E	214	LEU	3.6
1	E	526	TRP	3.6
1	E	579	VAL	3.6
1	F	385	LEU	3.6
1	G	153	VAL	3.6
1	I	525	TRP	3.6
1	K	371	LEU	3.6
1	K	383	TYR	3.6
1	L	464	LEU	3.6
1	A	168	LYS	3.6
1	A	397	LYS	3.6
1	D	386	LYS	3.6
1	B	555	SER	3.6
1	E	194	SER	3.6
1	J	548	SER	3.6
1	K	329	GLY	3.6
1	A	538	ASN	3.6
1	E	430	CYS	3.6
1	E	460	ALA	3.6
1	B	106	PRO	3.6
1	F	531	ASN	3.6
1	G	217	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
1	G	468	ASP	3.6
1	I	105	THR	3.6
1	K	276	THR	3.6
1	K	582	ASN	3.6
1	L	192	CYS	3.6
1	B	532	GLU	3.6
1	G	155	GLU	3.6
1	B	130	PHE	3.6
1	C	238	PHE	3.6
1	K	165	PHE	3.6
1	K	565	PHE	3.6
1	H	118	LYS	3.6
1	E	327	ILE	3.6
1	F	107	ILE	3.6
1	F	481	ILE	3.6
1	I	228	ILE	3.6
1	I	298	ILE	3.6
1	B	407	LEU	3.6
1	B	438	SER	3.6
1	B	541	TYR	3.6
1	C	263	TYR	3.6
1	E	207	VAL	3.6
1	E	325	TYR	3.6
1	E	328	LEU	3.6
1	F	359	TYR	3.6
1	H	411	TYR	3.6
1	I	350	TYR	3.6
1	L	593	VAL	3.6
1	E	381	GLY	3.6
1	C	279	GLU	3.6
1	E	155	GLU	3.6
1	B	440	ARG	3.6
1	E	585	ALA	3.6
1	L	300	ALA	3.6
1	J	417	LYS	3.6
1	A	252	PHE	3.6
1	B	583	PHE	3.6
1	E	238	PHE	3.6
1	K	425	PHE	3.6
1	A	86	SER	3.6
1	B	510	ILE	3.6
1	E	177	MET	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	167	VAL	3.6
1	D	262	GLU	3.6
1	G	576	ILE	3.6
1	H	94	LEU	3.6
1	H	391	SER	3.6
1	I	167	VAL	3.6
1	I	225	VAL	3.6
1	L	429	VAL	3.6
1	J	95	ASP	3.6
1	L	509	LEU	3.6
1	C	189	TYR	3.6
1	D	325	TYR	3.6
1	F	505	ASN	3.6
1	I	233	ASN	3.6
1	K	384	ASN	3.6
1	B	337	LYS	3.6
1	F	366	LYS	3.6
1	F	417	LYS	3.6
1	I	152	GLN	3.6
1	D	452	THR	3.6
1	E	307	PRO	3.6
1	H	212	THR	3.6
1	H	447	ALA	3.5
1	E	403	CYS	3.5
1	I	409	CYS	3.5
1	I	583	PHE	3.5
1	A	580	SER	3.5
1	B	580	SER	3.5
1	D	364	ASP	3.5
1	F	369	ILE	3.5
1	H	338	MET	3.5
1	I	578	GLY	3.5
1	K	140	GLY	3.5
1	C	413	VAL	3.5
1	E	371	LEU	3.5
1	F	207	VAL	3.5
1	J	157	LEU	3.5
1	K	323	LEU	3.5
1	L	217	ASN	3.5
1	G	288	TYR	3.5
1	K	439	TYR	3.5
1	C	89	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	404	ALA	3.5
1	C	291	THR	3.5
1	D	404	ALA	3.5
1	G	458	THR	3.5
1	I	404	ALA	3.5
1	J	452	THR	3.5
1	K	300	ALA	3.5
1	K	452	THR	3.5
1	B	215	HIS	3.5
1	D	331	LYS	3.5
1	A	501	GLY	3.5
1	D	179	ASN	3.5
1	F	295	SER	3.5
1	H	119	GLY	3.5
1	H	435	SER	3.5
1	C	378	PHE	3.5
1	H	289	PHE	3.5
1	I	149	ASN	3.5
1	L	462	GLY	3.5
1	C	349	MET	3.5
1	C	481	ILE	3.5
1	H	544	ILE	3.5
1	I	355	ILE	3.5
1	L	271	ILE	3.5
1	A	94	LEU	3.5
1	A	509	LEU	3.5
1	A	562	LEU	3.5
1	C	595	LEU	3.5
1	K	416	LEU	3.5
1	B	200	GLU	3.5
1	I	419	GLU	3.5
1	A	135	PRO	3.5
1	A	359	TYR	3.5
1	C	115	TYR	3.5
1	E	411	TYR	3.5
1	K	189	TYR	3.5
1	E	299	ALA	3.5
1	B	525	TRP	3.5
1	E	216	ASP	3.5
1	F	525	TRP	3.5
1	B	120	GLY	3.5
1	C	209	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	F	209	SER	3.5
1	I	98	SER	3.5
1	I	295	SER	3.5
1	I	498	SER	3.5
1	J	462	GLY	3.5
1	A	129	ILE	3.5
1	C	395	LEU	3.5
1	D	333	LEU	3.5
1	D	464	LEU	3.5
1	G	117	ILE	3.5
1	G	355	ILE	3.5
1	I	129	ILE	3.5
1	K	556	ILE	3.5
1	L	510	ILE	3.5
1	F	471	VAL	3.5
1	G	190	VAL	3.5
1	C	465	THR	3.5
1	D	597	THR	3.5
1	I	597	THR	3.5
1	K	314	ALA	3.5
1	L	541	TYR	3.5
1	G	215	HIS	3.5
1	L	181	ASN	3.5
1	B	550	SER	3.5
1	G	160	GLU	3.5
1	G	548	SER	3.5
1	G	571	TRP	3.5
1	H	580	SER	3.5
1	G	156	PHE	3.5
1	G	221	LYS	3.5
1	J	218	LYS	3.5
1	K	243	PHE	3.5
1	I	416	LEU	3.5
1	L	228	ILE	3.5
1	B	96	PRO	3.5
1	L	317	LEU	3.5
1	J	211	VAL	3.5
1	G	296	GLN	3.5
1	G	567	GLN	3.5
1	H	452	THR	3.5
1	I	291	THR	3.5
1	K	296	GLN	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	553	ALA	3.5
1	C	274	ALA	3.5
1	A	533	TYR	3.5
1	B	227	GLU	3.5
1	B	293	TYR	3.5
1	E	138	GLU	3.5
1	G	341	TYR	3.5
1	H	304	TYR	3.5
1	K	229	ASN	3.5
1	J	343	SER	3.5
1	J	501	GLY	3.5
1	L	343	SER	3.5
1	C	475	LYS	3.5
1	C	589	LYS	3.5
1	E	158	LYS	3.5
1	A	459	ASP	3.5
1	D	252	PHE	3.5
1	G	247	MET	3.5
1	K	213	MET	3.5
1	B	155	GLU	3.5
1	B	484	ILE	3.5
1	D	336	LEU	3.5
1	J	544	ILE	3.5
1	L	560	LEU	3.5
1	E	502	VAL	3.5
1	F	506	ASN	3.5
1	F	566	VAL	3.5
1	K	421	VAL	3.5
1	C	299	ALA	3.5
1	K	460	ALA	3.5
1	A	427	SER	3.5
1	C	86	SER	3.5
1	F	126	GLY	3.5
1	I	345	GLY	3.5
1	G	439	TYR	3.5
1	G	554	SER	3.5
1	I	520	SER	3.5
1	I	587	LYS	3.5
1	J	263	TYR	3.5
1	C	231	ASP	3.5
1	F	216	ASP	3.5
1	D	392	MET	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	599	PHE	3.4
1	H	89	PRO	3.4
1	A	355	ILE	3.4
1	B	99	ILE	3.4
1	B	342	LEU	3.4
1	B	530	ILE	3.4
1	D	129	ILE	3.4
1	E	129	ILE	3.4
1	F	131	LEU	3.4
1	G	556	ILE	3.4
1	K	470	LEU	3.4
1	L	407	LEU	3.4
1	L	547	ILE	3.4
1	C	362	LYS	3.4
1	E	377	THR	3.4
1	G	465	THR	3.4
1	I	551	VAL	3.4
1	J	132	VAL	3.4
1	J	232	LYS	3.4
1	L	362	LYS	3.4
1	J	391	SER	3.4
1	A	325	TYR	3.4
1	K	103	TYR	3.4
1	L	293	TYR	3.4
1	C	116	ASP	3.4
1	K	459	ASP	3.4
1	B	89	PRO	3.4
1	B	147	LYS	3.4
1	E	602	ASN	3.4
1	A	338	MET	3.4
1	A	354	PHE	3.4
1	B	97	THR	3.4
1	C	573	HIS	3.4
1	D	310	LEU	3.4
1	D	462	GLY	3.4
1	F	458	THR	3.4
1	G	501	GLY	3.4
1	I	241	THR	3.4
1	I	321	LEU	3.4
1	I	444	ILE	3.4
1	J	424	HIS	3.4
1	D	372	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	F	365	VAL	3.4
1	F	455	VAL	3.4
1	G	196	ALA	3.4
1	G	344	VAL	3.4
1	G	380	SER	3.4
1	G	455	VAL	3.4
1	H	194	SER	3.4
1	K	391	SER	3.4
1	K	467	ALA	3.4
1	L	124	GLU	3.4
1	L	269	VAL	3.4
1	I	515	GLN	3.4
1	C	159	ASP	3.4
1	C	325	TYR	3.4
1	H	115	TYR	3.4
1	H	265	LYS	3.4
1	J	304	TYR	3.4
1	K	278	LYS	3.4
1	A	420	ASN	3.4
1	F	133	ASN	3.4
1	H	420	ASN	3.4
1	E	441	PRO	3.4
1	A	268	GLY	3.4
1	A	465	THR	3.4
1	E	496	GLY	3.4
1	H	369	ILE	3.4
1	H	503	PHE	3.4
1	H	591	PHE	3.4
1	J	226	PHE	3.4
1	K	338	MET	3.4
1	L	477	GLY	3.4
1	A	184	SER	3.4
1	B	198	LEU	3.4
1	B	487	LEU	3.4
1	A	300	ALA	3.4
1	C	309	SER	3.4
1	C	549	SER	3.4
1	E	110	ILE	3.4
1	E	514	LEU	3.4
1	I	110	ILE	3.4
1	J	393	ILE	3.4
1	L	599	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	524	VAL	3.4
1	E	95	ASP	3.4
1	I	231	ASP	3.4
1	J	364	ASP	3.4
1	K	211	VAL	3.4
1	B	512	LYS	3.4
1	J	475	LYS	3.4
1	B	352	ASN	3.4
1	C	133	ASN	3.4
1	E	545	ASN	3.4
1	H	306	ASN	3.4
1	C	155	GLU	3.4
1	E	270	TYR	3.4
1	H	246	TYR	3.4
1	D	301	PRO	3.4
1	A	136	GLY	3.4
1	C	170	GLY	3.4
1	C	590	GLY	3.4
1	I	381	GLY	3.4
1	I	590	GLY	3.4
1	J	119	GLY	3.4
1	K	592	GLY	3.4
1	A	296	GLN	3.4
1	L	113	GLN	3.4
1	A	146	SER	3.4
1	B	451	LYS	3.4
1	E	209	SER	3.4
1	H	377	THR	3.4
1	I	458	THR	3.4
1	K	247	MET	3.4
1	C	201	ALA	3.4
1	C	527	LEU	3.4
1	F	284	ALA	3.4
1	J	562	LEU	3.4
1	K	317	LEU	3.4
1	B	571	TRP	3.4
1	H	434	VAL	3.4
1	H	581	TRP	3.4
1	J	167	VAL	3.4
1	G	511	ASN	3.4
1	H	316	GLU	3.4
1	H	508	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	I	229	ASN	3.4
1	J	511	ASN	3.4
1	A	588	PRO	3.4
1	G	456	GLY	3.4
1	G	109	ASP	3.4
1	C	491	MET	3.4
1	A	425	PHE	3.4
1	C	317	LEU	3.4
1	C	412	CYS	3.4
1	G	460	ALA	3.4
1	G	530	ILE	3.4
1	H	601	LEU	3.4
1	I	289	PHE	3.4
1	A	185	VAL	3.4
1	C	139	ASN	3.4
1	C	440	ARG	3.4
1	D	225	VAL	3.4
1	D	308	VAL	3.4
1	G	259	VAL	3.4
1	I	217	ASN	3.4
1	L	420	ASN	3.4
1	J	418	PRO	3.4
1	A	202	ASP	3.4
1	D	231	ASP	3.4
1	I	443	ASP	3.4
1	J	573	HIS	3.4
1	C	287	TYR	3.4
1	H	480	TYR	3.4
1	J	292	TYR	3.4
1	K	244	TYR	3.4
1	K	309	SER	3.4
1	K	555	SER	3.4
1	L	263	TYR	3.4
1	A	212	THR	3.4
1	L	248	THR	3.4
1	B	247	MET	3.4
1	B	400	MET	3.4
1	A	495	LEU	3.4
1	B	466	LEU	3.4
1	C	599	PHE	3.4
1	D	420	ASN	3.4
1	F	410	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	H	149	ASN	3.4
1	J	117	ILE	3.4
1	J	481	ILE	3.4
1	K	574	ILE	3.4
1	L	582	ASN	3.4
1	A	374	LYS	3.4
1	B	224	VAL	3.3
1	D	114	VAL	3.3
1	I	207	VAL	3.3
1	J	207	VAL	3.3
1	C	578	GLY	3.3
1	E	89	PRO	3.3
1	E	135	PRO	3.3
1	I	155	GLU	3.3
1	K	89	PRO	3.3
1	K	496	GLY	3.3
1	D	309	SER	3.3
1	K	209	SER	3.3
1	B	480	TYR	3.3
1	D	350	TYR	3.3
1	E	128	THR	3.3
1	F	415	THR	3.3
1	F	497	THR	3.3
1	I	439	TYR	3.3
1	I	569	THR	3.3
1	L	244	TYR	3.3
1	L	292	TYR	3.3
1	D	139	ASN	3.3
1	E	589	LYS	3.3
1	G	397	LYS	3.3
1	J	521	ASN	3.3
1	K	204	LYS	3.3
1	K	584	LYS	3.3
1	A	542	ALA	3.3
1	G	300	ALA	3.3
1	H	400	MET	3.3
1	B	560	LEU	3.3
1	C	214	LEU	3.3
1	E	198	LEU	3.3
1	E	297	LEU	3.3
1	H	527	LEU	3.3
1	I	336	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	561	PHE	3.3
1	F	530	ILE	3.3
1	G	481	ILE	3.3
1	E	334	GLU	3.3
1	F	102	GLU	3.3
1	B	190	VAL	3.3
1	D	230	VAL	3.3
1	G	114	VAL	3.3
1	K	372	VAL	3.3
1	K	429	VAL	3.3
1	A	193	GLY	3.3
1	D	489	GLY	3.3
1	K	121	CYS	3.3
1	L	496	GLY	3.3
1	I	360	LYS	3.3
1	D	465	THR	3.3
1	G	303	ASN	3.3
1	K	458	THR	3.3
1	A	244	TYR	3.3
1	B	493	TYR	3.3
1	J	325	TYR	3.3
1	C	558	ALA	3.3
1	G	388	ALA	3.3
1	L	196	ALA	3.3
1	B	231	ASP	3.3
1	H	231	ASP	3.3
1	C	110	ILE	3.3
1	D	175	PHE	3.3
1	D	271	ILE	3.3
1	G	453	ILE	3.3
1	J	453	ILE	3.3
1	K	228	ILE	3.3
1	L	243	PHE	3.3
1	D	373	GLY	3.3
1	H	408	GLY	3.3
1	D	365	VAL	3.3
1	F	224	VAL	3.3
1	J	372	VAL	3.3
1	A	594	ARG	3.3
1	F	312	ASN	3.3
1	A	474	GLU	3.3
1	J	571	TRP	3.3

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Mol	Chain	Res	Type	RSRZ
1	G	97	THR	3.3
1	I	536	THR	3.3
1	K	105	THR	3.3
1	K	497	THR	3.3
1	D	275	ASP	3.3
1	K	95	ASP	3.3
1	K	499	TYR	3.3
1	L	499	TYR	3.3
1	B	392	MET	3.3
1	D	349	MET	3.3
1	G	213	MET	3.3
1	B	242	LEU	3.3
1	C	560	LEU	3.3
1	C	562	LEU	3.3
1	I	368	LYS	3.3
1	J	560	LEU	3.3
1	K	501	GLY	3.3
1	J	175	PHE	3.3
1	L	369	ILE	3.3
1	H	266	HIS	3.3
1	B	295	SER	3.3
1	E	413	VAL	3.3
1	F	200	GLU	3.3
1	F	413	VAL	3.3
1	G	200	GLU	3.3
1	H	211	VAL	3.3
1	H	330	VAL	3.3
1	G	531	ASN	3.3
1	H	102	GLU	3.3
1	I	227	GLU	3.3
1	L	568	ASN	3.3
1	B	109	ASP	3.3
1	B	486	THR	3.3
1	J	379	ASP	3.3
1	J	465	THR	3.3
1	I	571	TRP	3.3
1	K	571	TRP	3.3
1	B	253	LYS	3.3
1	E	518	LYS	3.3
1	E	587	LYS	3.3
1	G	587	LYS	3.3
1	C	467	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	140	GLY	3.3
1	A	247	MET	3.3
1	B	533	TYR	3.3
1	F	439	TYR	3.3
1	F	590	GLY	3.3
1	G	463	ARG	3.3
1	H	402	GLY	3.3
1	H	456	GLY	3.3
1	I	341	TYR	3.3
1	H	282	GLU	3.3
1	A	327	ILE	3.3
1	B	481	ILE	3.3
1	C	264	ILE	3.3
1	C	271	ILE	3.3
1	E	591	PHE	3.3
1	F	547	ILE	3.3
1	I	445	ILE	3.3
1	K	235	PHE	3.3
1	B	516	SER	3.3
1	F	302	SER	3.3
1	G	233	ASN	3.3
1	J	181	ASN	3.3
1	G	182	LYS	3.3
1	I	362	LYS	3.3
1	G	446	THR	3.3
1	J	248	THR	3.3
1	A	284	ALA	3.3
1	A	373	GLY	3.3
1	B	375	GLY	3.3
1	C	489	GLY	3.3
1	C	585	ALA	3.3
1	D	485	ALA	3.3
1	G	192	CYS	3.3
1	L	428	ALA	3.3
1	A	411	TYR	3.3
1	E	162	MET	3.3
1	H	90	GLN	3.3
1	J	567	GLN	3.3
1	E	222	LEU	3.3
1	E	527	LEU	3.3
1	G	493	TYR	3.3
1	G	307	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
1	H	509	LEU	3.3
1	H	595	LEU	3.3
1	J	103	TYR	3.3
1	K	511	ASN	3.3
1	L	432	ASN	3.3
1	B	361	SER	3.3
1	B	238	PHE	3.3
1	B	376	ILE	3.3
1	E	98	SER	3.3
1	F	309	SER	3.3
1	F	380	SER	3.3
1	H	209	SER	3.3
1	J	530	ILE	3.3
1	K	516	SER	3.3
1	F	175	PHE	3.3
1	F	378	PHE	3.3
1	I	354	PHE	3.3
1	L	376	ILE	3.3
1	A	231	ASP	3.3
1	I	159	ASP	3.3
1	J	397	LYS	3.3
1	K	394	ASP	3.3
1	C	269	VAL	3.3
1	E	434	VAL	3.3
1	F	225	VAL	3.3
1	F	502	VAL	3.3
1	E	200	GLU	3.3
1	E	324	GLU	3.3
1	A	120	GLY	3.2
1	F	515	GLN	3.2
1	K	126	GLY	3.2
1	A	186	ALA	3.2
1	B	542	ALA	3.2
1	E	186	ALA	3.2
1	J	294	ALA	3.2
1	K	294	ALA	3.2
1	D	506	ASN	3.2
1	F	174	HIS	3.2
1	A	351	PRO	3.2
1	A	451	LYS	3.2
1	C	441	PRO	3.2
1	C	580	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	103	TYR	3.2
1	D	293	TYR	3.2
1	E	127	LEU	3.2
1	E	392	MET	3.2
1	G	168	LYS	3.2
1	H	253	LYS	3.2
1	A	493	TYR	3.2
1	F	86	SER	3.2
1	G	93	SER	3.2
1	G	328	LEU	3.2
1	H	309	SER	3.2
1	I	249	ASP	3.2
1	I	383	TYR	3.2
1	J	554	SER	3.2
1	K	341	TYR	3.2
1	K	537	LEU	3.2
1	L	194	SER	3.2
1	E	202	ASP	3.2
1	G	95	ASP	3.2
1	L	439	TYR	3.2
1	D	101	ILE	3.2
1	J	484	ILE	3.2
1	H	583	PHE	3.2
1	A	171	THR	3.2
1	H	105	THR	3.2
1	L	105	THR	3.2
1	E	462	GLY	3.2
1	E	374	LYS	3.2
1	K	253	LYS	3.2
1	L	168	LYS	3.2
1	A	122	ASN	3.2
1	A	258	ASN	3.2
1	A	370	ALA	3.2
1	C	388	ALA	3.2
1	D	217	ASN	3.2
1	D	558	ALA	3.2
1	C	438	SER	3.2
1	C	443	ASP	3.2
1	C	507	GLU	3.2
1	F	351	PRO	3.2
1	H	379	ASP	3.2
1	H	517	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	I	95	ASP	3.2
1	L	332	GLU	3.2
1	F	205	ARG	3.2
1	I	210	LEU	3.2
1	J	214	LEU	3.2
1	C	574	ILE	3.2
1	D	304	TYR	3.2
1	G	327	ILE	3.2
1	H	129	ILE	3.2
1	K	325	TYR	3.2
1	K	493	TYR	3.2
1	F	243	PHE	3.2
1	L	546	GLN	3.2
1	A	187	VAL	3.2
1	E	455	VAL	3.2
1	E	475	LYS	3.2
1	J	286	VAL	3.2
1	L	185	VAL	3.2
1	A	488	THR	3.2
1	B	128	THR	3.2
1	C	382	GLY	3.2
1	D	536	THR	3.2
1	B	104	ASN	3.2
1	G	437	ASN	3.2
1	I	602	ASN	3.2
1	E	431	GLU	3.2
1	H	507	GLU	3.2
1	G	405	ALA	3.2
1	J	370	ALA	3.2
1	C	184	SER	3.2
1	E	580	SER	3.2
1	F	307	PRO	3.2
1	F	389	PRO	3.2
1	B	213	MET	3.2
1	B	527	LEU	3.2
1	B	596	LEU	3.2
1	C	350	TYR	3.2
1	H	533	TYR	3.2
1	J	383	TYR	3.2
1	L	327	ILE	3.2
1	F	403	CYS	3.2
1	G	130	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	593	VAL	3.2
1	F	335	GLU	3.2
1	G	408	GLY	3.2
1	E	536	THR	3.2
1	I	429	VAL	3.2
1	G	231	ASP	3.2
1	F	311	SER	3.2
1	G	314	ALA	3.2
1	E	346	LYS	3.2
1	G	367	LYS	3.2
1	J	323	LEU	3.2
1	K	219	LEU	3.2
1	A	160	GLU	3.2
1	I	564	GLU	3.2
1	A	408	GLY	3.2
1	D	181	ASN	3.2
1	D	411	TYR	3.2
1	D	602	ASN	3.2
1	F	503	PHE	3.2
1	H	235	PHE	3.2
1	H	575	ASP	3.2
1	K	561	PHE	3.2
1	A	121	CYS	3.2
1	B	429	VAL	3.2
1	C	112	VAL	3.2
1	D	190	VAL	3.2
1	E	286	VAL	3.2
1	F	215	HIS	3.2
1	H	241	THR	3.2
1	H	372	VAL	3.2
1	L	97	THR	3.2
1	L	281	VAL	3.2
1	B	218	LYS	3.2
1	C	343	SER	3.2
1	G	220	SER	3.2
1	K	331	LYS	3.2
1	A	141	PRO	3.2
1	D	588	PRO	3.2
1	K	351	PRO	3.2
1	K	461	GLU	3.2
1	D	407	LEU	3.2
1	E	157	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	342	LEU	3.2
1	J	213	MET	3.2
1	K	214	LEU	3.2
1	K	349	MET	3.2
1	E	109	ASP	3.2
1	F	414	GLY	3.2
1	H	363	GLY	3.2
1	L	345	GLY	3.2
1	B	264	ILE	3.2
1	I	453	ILE	3.2
1	A	304	TYR	3.2
1	B	499	TYR	3.2
1	C	289	PHE	3.2
1	D	111	LYS	3.2
1	F	341	TYR	3.2
1	F	536	THR	3.2
1	H	518	LYS	3.2
1	I	356	HIS	3.2
1	J	451	LYS	3.2
1	J	597	THR	3.2
1	K	241	THR	3.2
1	K	386	LYS	3.2
1	A	567	GLN	3.2
1	E	566	VAL	3.2
1	H	557	VAL	3.2
1	K	413	VAL	3.2
1	F	98	SER	3.2
1	F	220	SER	3.2
1	H	448	SER	3.2
1	C	447	ALA	3.2
1	G	274	ALA	3.2
1	A	317	LEU	3.2
1	C	366	LYS	3.2
1	D	345	GLY	3.2
1	F	363	GLY	3.2
1	F	476	LEU	3.2
1	K	143	LYS	3.2
1	K	333	LEU	3.2
1	K	342	LEU	3.2
1	G	546	GLN	3.1
1	K	513	ILE	3.1
1	A	497	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	304	TYR	3.1
1	E	165	PHE	3.1
1	E	235	PHE	3.1
1	L	358	THR	3.1
1	L	458	THR	3.1
1	A	315	VAL	3.1
1	B	427	SER	3.1
1	D	380	SER	3.1
1	F	361	SER	3.1
1	J	499	TYR	3.1
1	G	225	VAL	3.1
1	K	187	VAL	3.1
1	B	428	ALA	3.1
1	F	460	ALA	3.1
1	I	588	PRO	3.1
1	C	437	ASN	3.1
1	F	192	CYS	3.1
1	F	231	ASP	3.1
1	I	337	LYS	3.1
1	J	137	LYS	3.1
1	J	180	ASP	3.1
1	L	512	LYS	3.1
1	G	339	GLY	3.1
1	C	567	GLN	3.1
1	E	422	GLU	3.1
1	K	262	GLU	3.1
1	F	495	LEU	3.1
1	I	297	LEU	3.1
1	K	198	LEU	3.1
1	K	476	LEU	3.1
1	L	349	MET	3.1
1	A	424	HIS	3.1
1	H	291	THR	3.1
1	H	519	THR	3.1
1	J	444	ILE	3.1
1	B	435	SER	3.1
1	C	398	PHE	3.1
1	D	145	SER	3.1
1	H	311	SER	3.1
1	J	398	PHE	3.1
1	A	344	VAL	3.1
1	C	301	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	91	VAL	3.1
1	I	326	LYS	3.1
1	K	176	TYR	3.1
1	B	186	ALA	3.1
1	D	299	ALA	3.1
1	F	387	ALA	3.1
1	H	294	ALA	3.1
1	I	440	ARG	3.1
1	H	531	ASN	3.1
1	J	149	ASN	3.1
1	A	245	GLU	3.1
1	B	191	GLY	3.1
1	D	456	GLY	3.1
1	C	596	LEU	3.1
1	G	177	MET	3.1
1	J	342	LEU	3.1
1	A	529	ILE	3.1
1	B	129	ILE	3.1
1	B	584	LYS	3.1
1	E	241	THR	3.1
1	G	486	THR	3.1
1	H	320	LYS	3.1
1	I	128	THR	3.1
1	J	107	ILE	3.1
1	K	199	SER	3.1
1	K	368	LYS	3.1
1	C	503	PHE	3.1
1	A	582	ASN	3.1
1	D	379	ASP	3.1
1	G	161	ASN	3.1
1	H	461	GLU	3.1
1	H	506	ASN	3.1
1	I	166	ASN	3.1
1	I	511	ASN	3.1
1	I	521	ASN	3.1
1	J	420	ASN	3.1
1	L	160	GLU	3.1
1	B	246	TYR	3.1
1	D	288	TYR	3.1
1	D	388	ALA	3.1
1	E	103	TYR	3.1
1	E	244	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	308	VAL	3.1
1	G	281	VAL	3.1
1	I	185	VAL	3.1
1	C	546	GLN	3.1
1	L	356	HIS	3.1
1	A	540	LYS	3.1
1	B	182	LYS	3.1
1	D	278	LYS	3.1
1	F	204	LYS	3.1
1	G	204	LYS	3.1
1	A	371	LEU	3.1
1	B	239	LEU	3.1
1	B	537	LEU	3.1
1	C	222	LEU	3.1
1	C	242	LEU	3.1
1	C	342	LEU	3.1
1	E	509	LEU	3.1
1	F	349	MET	3.1
1	A	102	GLU	3.1
1	A	559	SER	3.1
1	B	102	GLU	3.1
1	B	520	SER	3.1
1	C	427	SER	3.1
1	I	184	SER	3.1
1	I	554	SER	3.1
1	K	205	ARG	3.1
1	L	184	SER	3.1
1	A	479	ASP	3.1
1	C	241	THR	3.1
1	C	358	THR	3.1
1	D	358	THR	3.1
1	D	575	ASP	3.1
1	E	358	THR	3.1
1	J	97	THR	3.1
1	L	109	ASP	3.1
1	A	306	ASN	3.1
1	B	444	ILE	3.1
1	C	101	ILE	3.1
1	G	306	ASN	3.1
1	H	481	ILE	3.1
1	C	100	PRO	3.1
1	K	545	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	L	273	ASN	3.1
1	L	306	ASN	3.1
1	B	237	PHE	3.1
1	E	482	VAL	3.1
1	F	269	VAL	3.1
1	F	339	GLY	3.1
1	I	290	GLY	3.1
1	E	288	TYR	3.1
1	K	263	TYR	3.1
1	A	332	GLU	3.1
1	A	525	TRP	3.1
1	F	285	ARG	3.1
1	J	564	GLU	3.1
1	K	227	GLU	3.1
1	A	169	LEU	3.1
1	B	220	SER	3.1
1	D	214	LEU	3.1
1	E	323	LEU	3.1
1	I	343	SER	3.1
1	L	133	ASN	3.1
1	A	307	PRO	3.1
1	B	327	ILE	3.1
1	F	513	ILE	3.1
1	G	445	ILE	3.1
1	I	106	PRO	3.1
1	K	544	ILE	3.1
1	L	89	PRO	3.1
1	A	462	GLY	3.1
1	F	592	GLY	3.1
1	G	170	GLY	3.1
1	G	563	LYS	3.1
1	J	329	GLY	3.1
1	K	402	GLY	3.1
1	F	591	PHE	3.1
1	K	512	LYS	3.1
1	J	577	ALA	3.1
1	K	186	ALA	3.1
1	L	92	VAL	3.1
1	L	211	VAL	3.1
1	L	507	GLU	3.1
1	F	244	TYR	3.1
1	F	399	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	H	483	ASP	3.1
1	A	352	ASN	3.1
1	B	343	SER	3.1
1	E	104	ASN	3.1
1	E	539	SER	3.1
1	G	166	ASN	3.1
1	K	548	SER	3.1
1	C	223	THR	3.1
1	E	267	LEU	3.1
1	E	476	LEU	3.1
1	G	466	LEU	3.1
1	J	198	LEU	3.1
1	J	526	TRP	3.1
1	G	584	LYS	3.1
1	J	291	THR	3.1
1	E	170	GLY	3.1
1	H	430	CYS	3.1
1	H	576	ILE	3.1
1	I	544	ILE	3.1
1	J	382	GLY	3.1
1	K	290	GLY	3.1
1	E	473	ALA	3.1
1	I	235	PHE	3.1
1	L	500	ALA	3.1
1	C	455	VAL	3.0
1	D	281	VAL	3.0
1	D	573	HIS	3.0
1	J	524	VAL	3.0
1	C	480	TYR	3.0
1	F	350	TYR	3.0
1	K	411	TYR	3.0
1	K	546	GLN	3.0
1	A	166	ASN	3.0
1	A	309	SER	3.0
1	B	209	SER	3.0
1	C	554	SER	3.0
1	E	166	ASN	3.0
1	F	173	LYS	3.0
1	G	348	SER	3.0
1	H	332	GLU	3.0
1	I	127	LEU	3.0
1	K	279	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	K	377	THR	3.0
1	D	477	GLY	3.0
1	L	586	ARG	3.0
1	F	393	ILE	3.0
1	H	376	ILE	3.0
1	A	468	ASP	3.0
1	F	318	ALA	3.0
1	B	305	CYS	3.0
1	F	603	ASP	3.0
1	G	394	ASP	3.0
1	H	424	HIS	3.0
1	I	503	PHE	3.0
1	K	174	HIS	3.0
1	B	344	VAL	3.0
1	C	582	ASN	3.0
1	H	315	VAL	3.0
1	I	91	VAL	3.0
1	L	167	VAL	3.0
1	C	98	SER	3.0
1	C	498	SER	3.0
1	D	263	TYR	3.0
1	E	341	TYR	3.0
1	E	499	TYR	3.0
1	F	325	TYR	3.0
1	F	494	SER	3.0
1	G	332	GLU	3.0
1	I	361	SER	3.0
1	I	480	TYR	3.0
1	I	493	TYR	3.0
1	K	270	TYR	3.0
1	B	578	GLY	3.0
1	D	105	THR	3.0
1	D	381	GLY	3.0
1	F	96	PRO	3.0
1	I	323	LEU	3.0
1	L	396	MET	3.0
1	C	571	TRP	3.0
1	J	197	ASP	3.0
1	J	525	TRP	3.0
1	J	581	TRP	3.0
1	A	386	LYS	3.0
1	C	218	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	410	ALA	3.0
1	A	573	HIS	3.0
1	B	469	ALA	3.0
1	D	542	ALA	3.0
1	F	453	ILE	3.0
1	G	410	ALA	3.0
1	G	542	ALA	3.0
1	J	340	ALA	3.0
1	K	129	ILE	3.0
1	K	144	ILE	3.0
1	A	449	ASN	3.0
1	D	183	ASN	3.0
1	D	532	GLU	3.0
1	E	124	GLU	3.0
1	G	545	ASN	3.0
1	I	522	GLU	3.0
1	K	505	ASN	3.0
1	F	391	SER	3.0
1	I	269	VAL	3.0
1	I	309	SER	3.0
1	J	206	VAL	3.0
1	D	246	TYR	3.0
1	F	251	ARG	3.0
1	F	586	ARG	3.0
1	H	541	TYR	3.0
1	J	533	TYR	3.0
1	K	236	ARG	3.0
1	G	590	GLY	3.0
1	D	351	PRO	3.0
1	I	418	PRO	3.0
1	G	208	LEU	3.0
1	I	177	MET	3.0
1	L	118	LYS	3.0
1	E	113	GLN	3.0
1	I	575	ASP	3.0
1	L	416	LEU	3.0
1	C	316	GLU	3.0
1	G	598	GLU	3.0
1	J	422	GLU	3.0
1	C	544	ILE	3.0
1	D	144	ILE	3.0
1	E	313	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	571	TRP	3.0
1	F	228	ILE	3.0
1	G	553	ALA	3.0
1	H	298	ILE	3.0
1	I	322	ASN	3.0
1	I	352	ASN	3.0
1	K	107	ILE	3.0
1	J	252	PHE	3.0
1	J	494	SER	3.0
1	L	354	PHE	3.0
1	D	132	VAL	3.0
1	H	142	VAL	3.0
1	C	278	LYS	3.0
1	C	386	LYS	3.0
1	D	518	LYS	3.0
1	E	402	GLY	3.0
1	H	375	GLY	3.0
1	A	106	PRO	3.0
1	A	394	ASP	3.0
1	A	543	ASP	3.0
1	D	116	ASP	3.0
1	G	113	GLN	3.0
1	G	270	TYR	3.0
1	H	288	TYR	3.0
1	J	519	THR	3.0
1	K	359	TYR	3.0
1	L	325	TYR	3.0
1	C	203	MET	3.0
1	C	396	MET	3.0
1	D	131	LEU	3.0
1	D	342	LEU	3.0
1	E	242	LEU	3.0
1	F	357	LEU	3.0
1	C	215	HIS	3.0
1	C	306	ASN	3.0
1	G	181	ASN	3.0
1	G	573	HIS	3.0
1	H	312	ASN	3.0
1	B	285	ARG	3.0
1	B	387	ALA	3.0
1	F	370	ALA	3.0
1	C	520	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	539	SER	3.0
1	G	99	ILE	3.0
1	J	485	ALA	3.0
1	L	481	ILE	3.0
1	L	530	ILE	3.0
1	A	436	LYS	3.0
1	B	221	LYS	3.0
1	A	124	GLU	3.0
1	E	243	PHE	3.0
1	B	421	VAL	3.0
1	B	471	VAL	3.0
1	D	600	VAL	3.0
1	E	185	VAL	3.0
1	F	249	ASP	3.0
1	G	88	VAL	3.0
1	G	140	GLY	3.0
1	G	379	ASP	3.0
1	J	344	VAL	3.0
1	G	441	PRO	3.0
1	G	452	THR	3.0
1	I	89	PRO	3.0
1	J	486	THR	3.0
1	K	569	THR	3.0
1	C	430	CYS	3.0
1	D	292	TYR	3.0
1	E	192	CYS	3.0
1	A	131	LEU	3.0
1	D	509	LEU	3.0
1	I	239	LEU	3.0
1	L	104	ASN	3.0
1	C	594	ARG	3.0
1	A	151	LYS	3.0
1	B	254	SER	3.0
1	B	448	SER	3.0
1	C	300	ALA	3.0
1	C	448	SER	3.0
1	G	124	GLU	3.0
1	H	124	GLU	3.0
1	H	555	SER	3.0
1	I	405	ALA	3.0
1	K	448	SER	3.0
1	L	361	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	L	467	ALA	3.0
1	C	369	ILE	3.0
1	D	298	ILE	3.0
1	K	445	ILE	3.0
1	B	382	GLY	3.0
1	D	590	GLY	3.0
1	I	116	ASP	3.0
1	D	583	PHE	3.0
1	H	526	TRP	3.0
1	A	441	PRO	3.0
1	H	471	VAL	3.0
1	J	153	VAL	3.0
1	G	149	ASN	3.0
1	G	432	ASN	3.0
1	E	540	LYS	3.0
1	E	586	ARG	3.0
1	L	368	LYS	3.0
1	C	262	GLU	2.9
1	C	341	TYR	2.9
1	D	189	TYR	2.9
1	D	335	GLU	2.9
1	E	532	GLU	2.9
1	F	214	LEU	2.9
1	G	157	LEU	2.9
1	H	208	LEU	2.9
1	J	321	LEU	2.9
1	K	292	TYR	2.9
1	L	430	CYS	2.9
1	B	348	SER	2.9
1	C	318	ALA	2.9
1	F	490	ALA	2.9
1	J	559	SER	2.9
1	K	542	ALA	2.9
1	L	585	ALA	2.9
1	B	275	ASP	2.9
1	K	483	ASP	2.9
1	A	101	ILE	2.9
1	A	481	ILE	2.9
1	D	530	ILE	2.9
1	G	496	GLY	2.9
1	I	375	GLY	2.9
1	B	591	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	226	PHE	2.9
1	D	135	PRO	2.9
1	F	165	PHE	2.9
1	G	230	VAL	2.9
1	G	420	ASN	2.9
1	G	440	ARG	2.9
1	J	237	PHE	2.9
1	K	252	PHE	2.9
1	E	133	ASN	2.9
1	F	92	VAL	2.9
1	K	531	ASN	2.9
1	B	223	THR	2.9
1	D	491	MET	2.9
1	G	210	LEU	2.9
1	G	287	TYR	2.9
1	J	203	MET	2.9
1	J	350	TYR	2.9
1	J	464	LEU	2.9
1	L	385	LEU	2.9
1	B	399	ASP	2.9
1	D	109	ASP	2.9
1	D	435	SER	2.9
1	F	483	ASP	2.9
1	L	93	SER	2.9
1	B	490	ALA	2.9
1	D	473	ALA	2.9
1	E	572	ALA	2.9
1	L	447	ALA	2.9
1	L	553	ALA	2.9
1	F	381	GLY	2.9
1	G	430	CYS	2.9
1	K	120	GLY	2.9
1	C	374	LYS	2.9
1	E	228	ILE	2.9
1	I	574	ILE	2.9
1	L	205	ARG	2.9
1	C	233	ASN	2.9
1	C	568	ASN	2.9
1	G	183	ASN	2.9
1	A	238	PHE	2.9
1	B	356	HIS	2.9
1	K	226	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	413	VAL	2.9
1	E	315	VAL	2.9
1	G	207	VAL	2.9
1	K	600	VAL	2.9
1	H	525	TRP	2.9
1	J	483	ASP	2.9
1	A	548	SER	2.9
1	A	554	SER	2.9
1	E	145	SER	2.9
1	F	555	SER	2.9
1	G	495	LEU	2.9
1	J	220	SER	2.9
1	I	257	LYS	2.9
1	I	491	MET	2.9
1	K	239	LEU	2.9
1	C	191	GLY	2.9
1	C	345	GLY	2.9
1	B	463	ARG	2.9
1	C	522	GLU	2.9
1	E	388	ALA	2.9
1	F	469	ALA	2.9
1	H	250	GLU	2.9
1	H	558	ALA	2.9
1	I	325	TYR	2.9
1	J	541	TYR	2.9
1	J	205	ARG	2.9
1	B	420	ASN	2.9
1	C	104	ASN	2.9
1	C	521	ASN	2.9
1	D	384	ASN	2.9
1	D	545	ASN	2.9
1	E	481	ILE	2.9
1	I	307	PRO	2.9
1	L	523	PRO	2.9
1	B	113	GLN	2.9
1	G	108	HIS	2.9
1	A	226	PHE	2.9
1	E	252	PHE	2.9
1	J	130	PHE	2.9
1	K	543	ASP	2.9
1	F	283	LYS	2.9
1	A	138	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	522	GLU	2.9
1	C	559	SER	2.9
1	H	348	SER	2.9
1	K	86	SER	2.9
1	L	516	SER	2.9
1	L	549	SER	2.9
1	L	559	SER	2.9
1	A	590	GLY	2.9
1	F	416	LEU	2.9
1	H	285	ARG	2.9
1	H	329	GLY	2.9
1	H	590	GLY	2.9
1	I	402	GLY	2.9
1	I	470	LEU	2.9
1	I	594	ARG	2.9
1	J	338	MET	2.9
1	K	514	LEU	2.9
1	L	433	MET	2.9
1	B	103	TYR	2.9
1	B	284	ALA	2.9
1	C	485	ALA	2.9
1	D	340	ALA	2.9
1	D	359	TYR	2.9
1	D	533	TYR	2.9
1	E	467	ALA	2.9
1	E	538	ASN	2.9
1	G	505	ASN	2.9
1	H	272	ASN	2.9
1	K	472	TYR	2.9
1	D	99	ILE	2.9
1	E	107	ILE	2.9
1	I	301	PRO	2.9
1	L	423	ILE	2.9
1	H	95	ASP	2.9
1	K	446	THR	2.9
1	C	178	PHE	2.9
1	A	438	SER	2.9
1	A	555	SER	2.9
1	C	114	VAL	2.9
1	C	281	VAL	2.9
1	C	421	VAL	2.9
1	J	440	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	140	GLY	2.9
1	A	416	LEU	2.9
1	B	601	LEU	2.9
1	C	476	LEU	2.9
1	D	527	LEU	2.9
1	F	526	TRP	2.9
1	J	416	LEU	2.9
1	L	272	ASN	2.9
1	A	113	GLN	2.9
1	C	370	ALA	2.9
1	C	473	ALA	2.9
1	G	313	ALA	2.9
1	C	176	TYR	2.9
1	J	341	TYR	2.9
1	E	282	GLU	2.9
1	E	573	HIS	2.9
1	F	89	PRO	2.9
1	G	399	ASP	2.9
1	J	202	ASP	2.9
1	L	102	GLU	2.9
1	C	445	ILE	2.9
1	E	529	ILE	2.9
1	J	355	ILE	2.9
1	G	586	ARG	2.9
1	J	516	SER	2.9
1	L	554	SER	2.9
1	A	132	VAL	2.9
1	B	406	VAL	2.9
1	C	600	VAL	2.9
1	E	268	GLY	2.9
1	I	482	VAL	2.9
1	K	403	CYS	2.9
1	G	122	ASN	2.9
1	A	155	GLU	2.9
1	B	160	GLU	2.9
1	B	461	GLU	2.9
1	D	280	GLU	2.9
1	E	400	MET	2.9
1	F	467	ALA	2.9
1	I	186	ALA	2.9
1	I	219	LEU	2.9
1	I	313	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	J	131	LEU	2.9
1	J	407	LEU	2.9
1	E	468	ASP	2.9
1	F	109	ASP	2.9
1	C	266	HIS	2.9
1	D	441	PRO	2.9
1	E	263	TYR	2.9
1	F	541	TYR	2.9
1	D	510	ILE	2.8
1	D	291	THR	2.8
1	F	498	SER	2.8
1	G	241	THR	2.8
1	G	448	SER	2.8
1	H	559	SER	2.8
1	I	380	SER	2.8
1	I	391	SER	2.8
1	K	172	SER	2.8
1	A	126	GLY	2.8
1	A	178	PHE	2.8
1	B	360	LYS	2.8
1	B	503	PHE	2.8
1	E	183	ASN	2.8
1	E	303	ASN	2.8
1	E	432	ASN	2.8
1	G	538	ASN	2.8
1	H	188	GLY	2.8
1	F	451	LYS	2.8
1	H	218	LYS	2.8
1	I	531	ASN	2.8
1	J	457	ASN	2.8
1	L	218	LYS	2.8
1	D	406	VAL	2.8
1	G	125	GLU	2.8
1	L	413	VAL	2.8
1	L	305	CYS	2.8
1	C	433	MET	2.8
1	D	357	LEU	2.8
1	E	428	ALA	2.8
1	F	338	MET	2.8
1	G	476	LEU	2.8
1	H	299	ALA	2.8
1	H	467	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	H	491	MET	2.8
1	F	480	TYR	2.8
1	A	241	THR	2.8
1	C	283	LYS	2.8
1	D	296	GLN	2.8
1	D	529	ILE	2.8
1	E	452	THR	2.8
1	F	194	SER	2.8
1	F	401	SER	2.8
1	H	401	SER	2.8
1	H	563	LYS	2.8
1	K	271	ILE	2.8
1	L	555	SER	2.8
1	J	449	ASN	2.8
1	K	133	ASN	2.8
1	B	249	ASP	2.8
1	C	566	VAL	2.8
1	D	593	VAL	2.8
1	E	132	VAL	2.8
1	E	379	ASP	2.8
1	I	178	PHE	2.8
1	G	148	VAL	2.8
1	G	429	VAL	2.8
1	I	142	VAL	2.8
1	B	470	LEU	2.8
1	D	553	ALA	2.8
1	G	321	LEU	2.8
1	K	404	ALA	2.8
1	L	400	MET	2.8
1	G	232	LYS	2.8
1	J	278	LYS	2.8
1	A	270	TYR	2.8
1	A	499	TYR	2.8
1	C	375	GLY	2.8
1	C	391	SER	2.8
1	D	322	ASN	2.8
1	B	423	ILE	2.8
1	F	411	TYR	2.8
1	G	223	THR	2.8
1	G	510	ILE	2.8
1	I	246	TYR	2.8
1	I	559	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	J	154	SER	2.8
1	K	322	ASN	2.8
1	K	520	SER	2.8
1	L	435	SER	2.8
1	I	529	ILE	2.8
1	J	128	THR	2.8
1	K	212	THR	2.8
1	E	463	ARG	2.8
1	D	354	PHE	2.8
1	C	92	VAL	2.8
1	J	566	VAL	2.8
1	J	587	LYS	2.8
1	K	286	VAL	2.8
1	B	474	GLU	2.8
1	B	485	ALA	2.8
1	C	282	GLU	2.8
1	L	200	GLU	2.8
1	L	404	ALA	2.8
1	A	492	LEU	2.8
1	B	94	LEU	2.8
1	B	214	LEU	2.8
1	B	509	LEU	2.8
1	C	515	GLN	2.8
1	G	333	LEU	2.8
1	C	179	ASN	2.8
1	C	432	ASN	2.8
1	G	384	ASN	2.8
1	K	430	CYS	2.8
1	D	290	GLY	2.8
1	E	220	SER	2.8
1	E	477	GLY	2.8
1	H	295	SER	2.8
1	J	172	SER	2.8
1	J	414	GLY	2.8
1	K	462	GLY	2.8
1	L	375	GLY	2.8
1	A	128	THR	2.8
1	A	519	THR	2.8
1	C	105	THR	2.8
1	A	586	ARG	2.8
1	K	231	ASP	2.8
1	I	513	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	K	444	ILE	2.8
1	L	350	TYR	2.8
1	E	240	GLU	2.8
1	E	335	GLU	2.8
1	E	360	LYS	2.8
1	F	353	LYS	2.8
1	J	143	LYS	2.8
1	K	87	GLU	2.8
1	D	235	PHE	2.8
1	C	225	VAL	2.8
1	C	312	ASN	2.8
1	C	531	ASN	2.8
1	F	384	ASN	2.8
1	F	568	ASN	2.8
1	H	407	LEU	2.8
1	I	139	ASN	2.8
1	J	538	ASN	2.8
1	L	384	ASN	2.8
1	C	401	SER	2.8
1	F	390	GLY	2.8
1	H	290	GLY	2.8
1	I	348	SER	2.8
1	J	193	GLY	2.8
1	K	456	GLY	2.8
1	L	402	GLY	2.8
1	C	379	ASP	2.8
1	F	275	ASP	2.8
1	B	212	THR	2.8
1	B	386	LYS	2.8
1	C	368	LYS	2.8
1	D	250	GLU	2.8
1	F	598	GLU	2.8
1	H	415	THR	2.8
1	I	486	THR	2.8
1	K	474	GLU	2.8
1	L	262	GLU	2.8
1	C	277	TYR	2.8
1	I	176	TYR	2.8
1	J	423	ILE	2.8
1	L	152	GLN	2.8
1	J	503	PHE	2.8
1	C	259	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	K	123	VAL	2.8
1	L	233	ASN	2.8
1	D	205	ARG	2.8
1	D	371	LEU	2.8
1	E	197	ASP	2.8
1	E	483	ASP	2.8
1	F	208	LEU	2.8
1	F	348	SER	2.8
1	I	401	SER	2.8
1	I	508	GLU	2.8
1	J	204	LYS	2.8
1	J	311	SER	2.8
1	J	360	LYS	2.8
1	K	158	LYS	2.8
1	B	497	THR	2.8
1	C	128	THR	2.8
1	F	105	THR	2.8
1	G	403	CYS	2.8
1	B	287	TYR	2.8
1	F	108	HIS	2.8
1	G	103	TYR	2.8
1	G	293	TYR	2.8
1	G	359	TYR	2.8
1	I	359	TYR	2.8
1	K	350	TYR	2.8
1	K	424	HIS	2.8
1	B	449	ASN	2.8
1	E	149	ASN	2.8
1	G	506	ASN	2.8
1	A	283	LYS	2.8
1	B	278	LYS	2.8
1	A	190	VAL	2.7
1	A	570	ALA	2.7
1	D	102	GLU	2.8
1	E	87	GLU	2.8
1	G	216	ASP	2.7
1	G	226	PHE	2.7
1	L	279	GLU	2.8
1	L	316	GLU	2.8
1	I	112	VAL	2.7
1	J	347	GLY	2.7
1	J	502	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	L	405	ALA	2.7
1	B	329	GLY	2.7
1	D	580	SER	2.7
1	F	408	GLY	2.7
1	L	98	SER	2.7
1	F	333	LEU	2.7
1	F	392	MET	2.7
1	E	296	GLN	2.7
1	B	415	THR	2.7
1	C	377	THR	2.7
1	G	519	THR	2.7
1	C	217	ASN	2.7
1	G	218	LYS	2.7
1	G	423	ILE	2.7
1	H	545	ASN	2.7
1	H	587	LYS	2.7
1	L	111	LYS	2.7
1	L	538	ASN	2.7
1	D	483	ASP	2.7
1	G	304	TYR	2.7
1	A	98	SER	2.7
1	D	370	ALA	2.7
1	F	428	ALA	2.7
1	G	299	ALA	2.7
1	G	428	ALA	2.7
1	H	577	ALA	2.7
1	K	387	ALA	2.7
1	D	421	VAL	2.7
1	E	167	VAL	2.7
1	F	226	PHE	2.7
1	I	471	VAL	2.7
1	I	600	VAL	2.7
1	J	365	VAL	2.7
1	K	527	LEU	2.7
1	L	514	LEU	2.7
1	I	400	MET	2.7
1	L	392	MET	2.7
1	I	279	GLU	2.7
1	I	488	THR	2.7
1	A	273	ASN	2.7
1	B	303	ASN	2.7
1	G	568	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	483	ASP	2.7
1	K	197	ASP	2.7
1	A	450	GLY	2.7
1	B	100	PRO	2.7
1	D	115	TYR	2.7
1	E	501	GLY	2.7
1	H	307	PRO	2.7
1	J	140	GLY	2.7
1	B	152	GLN	2.7
1	B	570	ALA	2.7
1	D	194	SER	2.7
1	G	539	SER	2.7
1	K	304	TYR	2.7
1	E	447	ALA	2.7
1	J	314	ALA	2.7
1	C	130	PHE	2.7
1	D	226	PHE	2.7
1	D	571	TRP	2.7
1	E	175	PHE	2.7
1	B	334	GLU	2.7
1	B	507	GLU	2.7
1	F	334	GLU	2.7
1	G	353	LYS	2.7
1	F	222	LEU	2.7
1	H	222	LEU	2.7
1	J	242	LEU	2.7
1	J	333	LEU	2.7
1	J	601	LEU	2.7
1	L	328	LEU	2.7
1	A	213	MET	2.7
1	B	349	MET	2.7
1	I	433	MET	2.7
1	E	212	THR	2.7
1	E	597	THR	2.7
1	A	174	HIS	2.7
1	A	312	ASN	2.7
1	A	399	ASP	2.7
1	E	364	ASP	2.7
1	I	273	ASN	2.7
1	K	159	ASP	2.7
1	C	530	ILE	2.7
1	D	110	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	382	GLY	2.7
1	J	327	ILE	2.7
1	J	339	GLY	2.7
1	K	453	ILE	2.7
1	C	96	PRO	2.7
1	D	143	LYS	2.7
1	E	353	LYS	2.7
1	I	507	GLU	2.7
1	J	337	LYS	2.7
1	J	362	LYS	2.7
1	K	431	GLU	2.7
1	K	508	GLU	2.7
1	B	383	TYR	2.7
1	D	287	TYR	2.7
1	J	318	ALA	2.7
1	J	359	TYR	2.7
1	L	103	TYR	2.7
1	A	175	PHE	2.7
1	B	478	VAL	2.7
1	D	142	VAL	2.7
1	D	463	ARG	2.7
1	A	336	LEU	2.7
1	A	432	ASN	2.7
1	A	505	ASN	2.7
1	C	336	LEU	2.7
1	F	305	CYS	2.7
1	G	185	VAL	2.7
1	H	593	VAL	2.7
1	J	91	VAL	2.7
1	K	112	VAL	2.7
1	L	175	PHE	2.7
1	F	545	ASN	2.7
1	H	426	LEU	2.7
1	L	596	LEU	2.7
1	G	364	ASP	2.7
1	I	223	THR	2.7
1	I	394	ASP	2.7
1	I	519	THR	2.7
1	K	171	THR	2.7
1	K	433	MET	2.7
1	L	497	THR	2.7
1	L	567	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	87	GLU	2.7
1	F	191	GLY	2.7
1	G	290	GLY	2.7
1	H	268	GLY	2.7
1	I	390	GLY	2.7
1	A	199	SER	2.7
1	G	98	SER	2.7
1	H	530	ILE	2.7
1	B	500	ALA	2.7
1	B	535	ALA	2.7
1	D	585	ALA	2.7
1	I	535	ALA	2.7
1	J	404	ALA	2.7
1	D	499	TYR	2.7
1	L	304	TYR	2.7
1	C	123	VAL	2.7
1	C	425	PHE	2.7
1	B	138	GLU	2.7
1	B	250	GLU	2.7
1	B	452	THR	2.7
1	C	169	LEU	2.7
1	C	187	VAL	2.7
1	C	328	LEU	2.7
1	D	153	VAL	2.7
1	G	237	PHE	2.7
1	J	561	PHE	2.7
1	K	156	PHE	2.7
1	E	424	HIS	2.7
1	F	514	LEU	2.7
1	K	478	VAL	2.7
1	G	316	GLU	2.7
1	H	515	GLN	2.7
1	I	232	LYS	2.7
1	J	124	GLU	2.7
1	J	162	MET	2.7
1	K	162	MET	2.7
1	E	525	TRP	2.7
1	L	456	GLY	2.7
1	A	516	SER	2.7
1	K	145	SER	2.7
1	L	96	PRO	2.7
1	L	440	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	L	463	ARG	2.7
1	B	547	ILE	2.7
1	D	444	ILE	2.7
1	H	355	ILE	2.7
1	K	110	ILE	2.7
1	E	405	ALA	2.7
1	C	449	ASN	2.7
1	G	459	ASP	2.7
1	L	521	ASN	2.7
1	L	575	ASP	2.7
1	C	461	GLU	2.7
1	D	218	LYS	2.7
1	F	218	LYS	2.7
1	G	374	LYS	2.7
1	G	411	TYR	2.7
1	I	113	GLN	2.7
1	J	293	TYR	2.7
1	K	552	LYS	2.7
1	A	478	VAL	2.7
1	A	527	LEU	2.7
1	B	357	LEU	2.7
1	F	310	LEU	2.7
1	J	330	VAL	2.7
1	F	400	MET	2.7
1	L	203	MET	2.7
1	I	136	GLY	2.7
1	J	592	GLY	2.7
1	L	590	GLY	2.7
1	A	251	ARG	2.6
1	A	440	ARG	2.6
1	K	539	SER	2.6
1	K	580	SER	2.6
1	L	525	TRP	2.6
1	B	307	PRO	2.6
1	E	301	PRO	2.6
1	L	301	PRO	2.6
1	A	249	ASP	2.6
1	C	240	GLU	2.6
1	D	161	ASN	2.6
1	D	306	ASN	2.6
1	H	164	LYS	2.6
1	H	384	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	I	122	ASN	2.6
1	I	327	ILE	2.6
1	J	179	ASN	2.6
1	J	510	ILE	2.6
1	F	500	ALA	2.6
1	L	201	ALA	2.6
1	A	189	TYR	2.6
1	A	595	LEU	2.6
1	B	593	VAL	2.6
1	C	458	THR	2.6
1	D	140	GLY	2.6
1	D	566	VAL	2.6
1	D	595	LEU	2.6
1	G	377	THR	2.6
1	G	497	THR	2.6
1	G	373	GLY	2.6
1	I	222	LEU	2.6
1	I	415	THR	2.6
1	J	345	GLY	2.6
1	J	463	ARG	2.6
1	J	487	LEU	2.6
1	L	212	THR	2.6
1	I	251	ARG	2.6
1	L	347	GLY	2.6
1	L	562	LEU	2.6
1	A	431	GLU	2.6
1	A	461	GLU	2.6
1	B	401	SER	2.6
1	D	334	GLU	2.6
1	E	227	GLU	2.6
1	F	554	SER	2.6
1	I	124	GLU	2.6
1	E	459	ASP	2.6
1	F	95	ASP	2.6
1	J	100	PRO	2.6
1	K	141	PRO	2.6
1	L	202	ASP	2.6
1	B	526	TRP	2.6
1	E	305	CYS	2.6
1	D	577	ALA	2.6
1	E	542	ALA	2.6
1	G	370	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	570	ALA	2.6
1	I	467	ALA	2.6
1	J	201	ALA	2.6
1	C	174	HIS	2.6
1	B	377	THR	2.6
1	B	536	THR	2.6
1	E	363	GLY	2.6
1	G	477	GLY	2.6
1	A	157	LEU	2.6
1	B	208	LEU	2.6
1	C	304	TYR	2.6
1	E	321	LEU	2.6
1	E	583	PHE	2.6
1	F	599	PHE	2.6
1	G	165	PHE	2.6
1	G	383	TYR	2.6
1	G	472	TYR	2.6
1	G	507	GLU	2.6
1	H	244	TYR	2.6
1	H	359	TYR	2.6
1	I	599	PHE	2.6
1	J	151	LYS	2.6
1	K	167	VAL	2.6
1	K	178	PHE	2.6
1	B	86	SER	2.6
1	B	494	SER	2.6
1	C	468	ASP	2.6
1	E	199	SER	2.6
1	F	433	MET	2.6
1	G	172	SER	2.6
1	K	438	SER	2.6
1	K	491	MET	2.6
1	L	479	ASP	2.6
1	F	546	GLN	2.6
1	J	89	PRO	2.6
1	J	588	PRO	2.6
1	D	440	ARG	2.6
1	E	564	GLU	2.6
1	I	282	GLU	2.6
1	L	163	GLU	2.6
1	L	245	GLU	2.6
1	C	339	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	504	GLY	2.6
1	I	592	GLY	2.6
1	A	97	THR	2.6
1	B	483	ASP	2.6
1	B	434	VAL	2.6
1	C	190	VAL	2.6
1	E	184	SER	2.6
1	G	86	SER	2.6
1	H	287	TYR	2.6
1	H	323	LEU	2.6
1	J	146	SER	2.6
1	K	246	TYR	2.6
1	L	309	SER	2.6
1	H	582	ASN	2.6
1	C	125	GLU	2.6
1	C	463	ARG	2.6
1	F	463	ARG	2.6
1	G	240	GLU	2.6
1	I	240	GLU	2.6
1	H	360	LYS	2.6
1	J	346	LYS	2.6
1	K	173	LYS	2.6
1	C	500	ALA	2.6
1	I	284	ALA	2.6
1	F	355	ILE	2.6
1	F	510	ILE	2.6
1	E	456	GLY	2.6
1	G	578	GLY	2.6
1	H	170	GLY	2.6
1	J	188	GLY	2.6
1	A	216	ASP	2.6
1	D	403	CYS	2.6
1	E	575	ASP	2.6
1	H	543	ASP	2.6
1	L	543	ASP	2.6
1	E	105	THR	2.6
1	J	152	GLN	2.6
1	A	343	SER	2.6
1	F	511	ASN	2.6
1	I	199	SER	2.6
1	J	309	SER	2.6
1	A	482	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	178	PHE	2.6
1	G	418	PRO	2.6
1	G	163	GLU	2.6
1	H	344	VAL	2.6
1	H	482	VAL	2.6
1	I	425	PHE	2.6
1	I	523	PRO	2.6
1	K	354	PHE	2.6
1	L	441	PRO	2.6
1	B	163	GLU	2.6
1	F	103	TYR	2.6
1	C	204	LYS	2.6
1	C	512	LYS	2.6
1	F	512	LYS	2.6
1	G	534	ARG	2.6
1	I	218	LYS	2.6
1	K	265	LYS	2.6
1	B	473	ALA	2.6
1	C	126	GLY	2.6
1	F	294	ALA	2.6
1	C	216	ASP	2.6
1	D	95	ASP	2.6
1	F	496	GLY	2.6
1	G	284	ALA	2.6
1	H	319	GLN	2.6
1	I	504	GLY	2.6
1	K	284	ALA	2.6
1	L	572	ALA	2.6
1	B	529	ILE	2.6
1	D	260	ASN	2.6
1	D	538	ASN	2.6
1	E	97	THR	2.6
1	J	139	ASN	2.6
1	K	134	ASN	2.6
1	E	555	SER	2.6
1	F	548	SER	2.6
1	G	438	SER	2.6
1	H	86	SER	2.6
1	H	160	GLU	2.6
1	K	532	GLU	2.6
1	B	204	LYS	2.6
1	E	436	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	I	436	LYS	2.6
1	B	317	LEU	2.6
1	F	336	LEU	2.6
1	G	106	PRO	2.6
1	K	357	LEU	2.6
1	B	338	MET	2.6
1	C	235	PHE	2.6
1	K	277	TYR	2.6
1	E	174	HIS	2.6
1	G	424	HIS	2.6
1	I	543	ASP	2.6
1	E	340	ALA	2.6
1	E	387	ALA	2.6
1	I	447	ALA	2.6
1	J	496	GLY	2.6
1	B	111	LYS	2.6
1	D	360	LYS	2.6
1	I	540	LYS	2.6
1	K	589	LYS	2.6
1	B	358	THR	2.5
1	D	172	SER	2.5
1	F	236	ARG	2.5
1	G	105	THR	2.5
1	K	528	PRO	2.5
1	A	476	LEU	2.5
1	C	357	LEU	2.5
1	A	177	MET	2.5
1	B	319	GLN	2.5
1	F	91	VAL	2.5
1	G	566	VAL	2.5
1	H	92	VAL	2.5
1	J	177	MET	2.5
1	L	213	MET	2.5
1	L	226	PHE	2.5
1	F	250	GLU	2.5
1	I	170	GLY	2.5
1	J	522	GLU	2.5
1	B	151	LYS	2.5
1	C	182	LYS	2.5
1	A	340	ALA	2.5
1	A	457	ASN	2.5
1	B	506	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	300	ALA	2.5
1	H	404	ALA	2.5
1	I	568	ASN	2.5
1	I	570	ALA	2.5
1	J	545	ASN	2.5
1	K	585	ALA	2.5
1	A	534	ARG	2.5
1	K	285	ARG	2.5
1	A	209	SER	2.5
1	E	86	SER	2.5
1	E	154	SER	2.5
1	F	520	SER	2.5
1	J	93	SER	2.5
1	L	401	SER	2.5
1	D	212	THR	2.5
1	E	248	THR	2.5
1	G	100	PRO	2.5
1	A	508	GLU	2.5
1	C	487	LEU	2.5
1	D	526	TRP	2.5
1	E	131	LEU	2.5
1	F	210	LEU	2.5
1	F	422	GLU	2.5
1	G	371	LEU	2.5
1	H	394	ASP	2.5
1	A	158	LYS	2.5
1	A	349	MET	2.5
1	A	368	LYS	2.5
1	A	413	VAL	2.5
1	A	491	MET	2.5
1	A	512	LYS	2.5
1	B	354	PHE	2.5
1	D	167	VAL	2.5
1	E	563	LYS	2.5
1	G	503	PHE	2.5
1	H	286	VAL	2.5
1	I	164	LYS	2.5
1	I	190	VAL	2.5
1	J	147	LYS	2.5
1	K	281	VAL	2.5
1	D	383	TYR	2.5
1	D	500	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	348	SER	2.5
1	F	438	SER	2.5
1	K	194	SER	2.5
1	C	519	THR	2.5
1	I	556	ILE	2.5
1	J	497	THR	2.5
1	K	97	THR	2.5
1	B	567	GLN	2.5
1	D	282	GLU	2.5
1	H	100	PRO	2.5
1	H	240	GLU	2.5
1	J	296	GLN	2.5
1	K	180	ASP	2.5
1	K	418	PRO	2.5
1	B	587	LYS	2.5
1	C	360	LYS	2.5
1	C	552	LYS	2.5
1	D	374	LYS	2.5
1	A	347	GLY	2.5
1	B	169	LEU	2.5
1	K	321	LEU	2.5
1	L	266	HIS	2.5
1	D	126	GLY	2.5
1	G	191	GLY	2.5
1	D	213	MET	2.5
1	D	437	ASN	2.5
1	E	225	VAL	2.5
1	H	303	ASN	2.5
1	H	600	VAL	2.5
1	J	225	VAL	2.5
1	K	183	ASN	2.5
1	F	313	ALA	2.5
1	L	186	ALA	2.5
1	A	564	GLU	2.5
1	E	461	GLU	2.5
1	I	151	LYS	2.5
1	I	296	GLN	2.5
1	J	386	LYS	2.5
1	K	374	LYS	2.5
1	F	128	THR	2.5
1	I	216	ASP	2.5
1	H	528	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	I	215	HIS	2.5
1	B	306	ASN	2.5
1	C	511	ASN	2.5
1	E	408	GLY	2.5
1	H	504	GLY	2.5
1	H	505	ASN	2.5
1	I	306	ASN	2.5
1	K	181	ASN	2.5
1	I	464	LEU	2.5
1	D	503	PHE	2.5
1	F	565	PHE	2.5
1	B	296	GLN	2.5
1	F	584	LYS	2.5
1	I	346	LYS	2.5
1	I	546	GLN	2.5
1	K	318	ALA	2.5
1	D	459	ASP	2.5
1	E	533	TYR	2.5
1	H	350	TYR	2.5
1	J	246	TYR	2.5
1	B	445	ILE	2.5
1	D	568	ASN	2.5
1	H	442	GLY	2.5
1	C	208	LEU	2.5
1	G	366	LYS	2.5
1	G	527	LEU	2.5
1	I	267	LEU	2.5
1	D	400	MET	2.5
1	F	213	MET	2.5
1	D	220	SER	2.5
1	E	224	VAL	2.5
1	F	468	ASP	2.5
1	G	482	VAL	2.5
1	I	315	VAL	2.5
1	D	525	TRP	2.5
1	H	370	ALA	2.5
1	I	585	ALA	2.5
1	B	244	TYR	2.5
1	D	128	THR	2.5
1	E	189	TYR	2.5
1	E	439	TYR	2.5
1	H	248	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	L	288	TYR	2.5
1	L	411	TYR	2.5
1	K	124	GLU	2.5
1	C	120	GLY	2.5
1	D	253	LYS	2.5
1	E	423	ILE	2.5
1	H	221	LYS	2.5
1	I	552	LYS	2.5
1	J	290	GLY	2.5
1	F	94	LEU	2.5
1	I	342	LEU	2.5
1	I	476	LEU	2.5
1	A	302	SER	2.4
1	D	427	SER	2.4
1	H	380	SER	2.4
1	I	427	SER	2.4
1	K	380	SER	2.4
1	A	421	VAL	2.4
1	D	206	VAL	2.4
1	D	251	ARG	2.4
1	G	251	ARG	2.4
1	C	245	GLU	2.4
1	D	572	ALA	2.4
1	K	130	PHE	2.4
1	J	461	GLU	2.4
1	K	370	ALA	2.4
1	D	446	THR	2.4
1	E	582	ASN	2.4
1	F	303	ASN	2.4
1	J	307	PRO	2.4
1	K	449	ASN	2.4
1	K	526	TRP	2.4
1	L	204	LYS	2.4
1	K	345	GLY	2.4
1	D	515	GLN	2.4
1	A	575	ASP	2.4
1	G	305	CYS	2.4
1	D	586	ARG	2.4
1	C	454	GLU	2.4
1	D	127	LEU	2.4
1	E	280	GLU	2.4
1	F	431	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	509	LEU	2.4
1	C	213	MET	2.4
1	D	204	LYS	2.4
1	D	540	LYS	2.4
1	E	338	MET	2.4
1	G	349	MET	2.4
1	H	552	LYS	2.4
1	I	278	LYS	2.4
1	A	237	PHE	2.4
1	A	502	VAL	2.4
1	D	165	PHE	2.4
1	D	413	VAL	2.4
1	G	572	ALA	2.4
1	J	142	VAL	2.4
1	J	313	ALA	2.4
1	J	447	ALA	2.4
1	K	225	VAL	2.4
1	F	166	ASN	2.4
1	I	104	ASN	2.4
1	I	432	ASN	2.4
1	A	301	PRO	2.4
1	B	441	PRO	2.4
1	B	170	GLY	2.4
1	C	456	GLY	2.4
1	I	191	GLY	2.4
1	I	266	HIS	2.4
1	L	446	THR	2.4
1	C	472	TYR	2.4
1	D	522	GLU	2.4
1	F	262	GLU	2.4
1	G	228	ILE	2.4
1	J	155	GLU	2.4
1	K	463	ARG	2.4
1	K	529	ILE	2.4
1	F	448	SER	2.4
1	G	494	SER	2.4
1	G	517	SER	2.4
1	H	438	SER	2.4
1	J	158	LYS	2.4
1	K	343	SER	2.4
1	A	514	LEU	2.4
1	I	192	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	531	ASN	2.4
1	F	521	ASN	2.4
1	I	338	MET	2.4
1	I	449	ASN	2.4
1	C	570	ALA	2.4
1	E	201	ALA	2.4
1	G	490	ALA	2.4
1	G	515	GLN	2.4
1	K	201	ALA	2.4
1	B	455	VAL	2.4
1	B	561	PHE	2.4
1	B	573	HIS	2.4
1	C	156	PHE	2.4
1	C	175	PHE	2.4
1	D	130	PHE	2.4
1	H	413	VAL	2.4
1	J	434	VAL	2.4
1	K	92	VAL	2.4
1	A	223	THR	2.4
1	E	590	GLY	2.4
1	I	446	THR	2.4
1	J	223	THR	2.4
1	J	241	THR	2.4
1	J	569	THR	2.4
1	L	290	GLY	2.4
1	B	236	ARG	2.4
1	C	102	GLU	2.4
1	C	474	GLU	2.4
1	K	594	ARG	2.4
1	F	278	LYS	2.4
1	E	444	ILE	2.4
1	F	544	ILE	2.4
1	G	369	ILE	2.4
1	I	481	ILE	2.4
1	L	110	ILE	2.4
1	I	86	SER	2.4
1	L	86	SER	2.4
1	K	242	LEU	2.4
1	C	390	GLY	2.4
1	C	572	ALA	2.4
1	D	240	GLU	2.4
1	D	247	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	553	ALA	2.4
1	G	489	GLY	2.4
1	H	579	VAL	2.4
1	I	389	PRO	2.4
1	I	489	GLY	2.4
1	K	215	HIS	2.4
1	K	473	ALA	2.4
1	D	156	PHE	2.4
1	D	479	ASP	2.4
1	E	164	LYS	2.4
1	I	586	ARG	2.4
1	J	212	THR	2.4
1	J	536	THR	2.4
1	A	93	SER	2.4
1	E	254	SER	2.4
1	E	516	SER	2.4
1	F	288	TYR	2.4
1	F	427	SER	2.4
1	F	580	SER	2.4
1	K	288	TYR	2.4
1	L	209	SER	2.4
1	B	544	ILE	2.4
1	A	303	ASN	2.4
1	E	90	GLN	2.4
1	E	125	GLU	2.4
1	I	324	GLU	2.4
1	K	125	GLU	2.4
1	A	596	LEU	2.4
1	I	395	LEU	2.4
1	L	267	LEU	2.4
1	B	408	GLY	2.4
1	E	159	ASP	2.4
1	E	173	LYS	2.4
1	H	109	ASP	2.4
1	H	459	ASP	2.4
1	H	592	GLY	2.4
1	J	285	ARG	2.4
1	J	500	ALA	2.4
1	K	347	GLY	2.4
1	K	475	LYS	2.4
1	L	151	LYS	2.4
1	K	553	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	L	249	ASP	2.4
1	L	339	GLY	2.4
1	L	436	LYS	2.4
1	I	314	ALA	2.4
1	L	570	ALA	2.4
1	L	573	HIS	2.4
1	D	96	PRO	2.4
1	B	206	VAL	2.4
1	H	566	VAL	2.4
1	K	536	THR	2.4
1	L	524	VAL	2.4
1	D	517	SER	2.4
1	G	319	GLN	2.4
1	K	494	SER	2.4
1	E	179	ASN	2.4
1	A	320	LYS	2.4
1	A	337	LYS	2.4
1	C	499	TYR	2.4
1	D	346	LYS	2.4
1	D	481	ILE	2.4
1	E	530	ILE	2.4
1	K	397	LYS	2.4
1	F	379	ASP	2.4
1	K	586	ARG	2.4
1	F	489	GLY	2.4
1	K	193	GLY	2.4
1	B	210	LEU	2.4
1	C	198	LEU	2.4
1	J	357	LEU	2.4
1	K	169	LEU	2.4
1	L	595	LEU	2.4
1	I	141	PRO	2.4
1	J	351	PRO	2.4
1	F	247	MET	2.4
1	J	433	MET	2.4
1	I	248	THR	2.4
1	A	163	GLU	2.4
1	D	112	VAL	2.4
1	D	482	VAL	2.4
1	E	142	VAL	2.4
1	K	132	VAL	2.4
1	D	199	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	361	SER	2.4
1	H	412	CYS	2.4
1	E	147	LYS	2.3
1	J	133	ASN	2.4
1	J	182	LYS	2.3
1	L	602	ASN	2.4
1	H	251	ARG	2.3
1	F	445	ILE	2.3
1	G	513	ILE	2.3
1	B	414	GLY	2.3
1	C	108	HIS	2.3
1	E	126	GLY	2.3
1	E	350	TYR	2.3
1	J	288	TYR	2.3
1	A	328	LEU	2.3
1	D	328	LEU	2.3
1	E	389	PRO	2.3
1	H	300	ALA	2.3
1	J	332	GLU	2.3
1	K	222	LEU	2.3
1	K	267	LEU	2.3
1	K	507	GLU	2.3
1	K	523	PRO	2.3
1	L	469	ALA	2.3
1	D	265	LYS	2.3
1	F	147	LYS	2.3
1	H	488	THR	2.3
1	I	518	LYS	2.3
1	A	114	VAL	2.3
1	A	217	ASN	2.3
1	C	272	ASN	2.3
1	G	502	VAL	2.3
1	J	295	SER	2.3
1	L	302	SER	2.3
1	L	517	SER	2.3
1	B	442	GLY	2.3
1	D	329	GLY	2.3
1	H	382	GLY	2.3
1	J	402	GLY	2.3
1	L	598	GLU	2.3
1	D	158	LYS	2.3
1	E	552	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	89	PRO	2.3
1	B	577	ALA	2.3
1	C	267	LEU	2.3
1	C	371	LEU	2.3
1	G	500	ALA	2.3
1	H	342	LEU	2.3
1	J	366	LYS	2.3
1	K	563	LYS	2.3
1	E	314	ALA	2.3
1	L	542	ALA	2.3
1	A	463	ARG	2.3
1	D	569	THR	2.3
1	E	233	ASN	2.3
1	G	203	MET	2.3
1	H	437	ASN	2.3
1	J	134	ASN	2.3
1	A	498	SER	2.3
1	B	502	VAL	2.3
1	C	249	ASP	2.3
1	D	249	ASP	2.3
1	E	435	SER	2.3
1	F	199	SER	2.3
1	B	454	GLU	2.3
1	I	125	GLU	2.3
1	I	461	GLU	2.3
1	L	227	GLU	2.3
1	A	170	GLY	2.3
1	C	373	GLY	2.3
1	I	462	GLY	2.3
1	K	366	LYS	2.3
1	K	436	LYS	2.3
1	C	409	CYS	2.3
1	D	513	ILE	2.3
1	H	418	PRO	2.3
1	A	333	LEU	2.3
1	C	538	ASN	2.3
1	J	371	LEU	2.3
1	J	472	TYR	2.3
1	K	480	TYR	2.3
1	K	568	ASN	2.3
1	A	282	GLU	2.3
1	C	380	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	348	SER	2.3
1	J	247	MET	2.3
1	L	483	ASP	2.3
1	J	200	GLU	2.3
1	K	330	VAL	2.3
1	L	232	LYS	2.3
1	L	482	VAL	2.3
1	B	126	GLY	2.3
1	D	193	GLY	2.3
1	I	319	GLN	2.3
1	J	373	GLY	2.3
1	G	529	ILE	2.3
1	L	588	PRO	2.3
1	C	303	ASN	2.3
1	H	535	ALA	2.3
1	J	507	GLU	2.3
1	C	470	LEU	2.3
1	G	302	SER	2.3
1	C	353	LYS	2.3
1	G	400	MET	2.3
1	G	433	MET	2.3
1	I	203	MET	2.3
1	F	329	GLY	2.3
1	H	126	GLY	2.3
1	H	339	GLY	2.3
1	L	108	HIS	2.3
1	L	238	PHE	2.3
1	L	308	VAL	2.3
1	C	384	ASN	2.3
1	H	454	GLU	2.3
1	L	166	ASN	2.3
1	A	475	LYS	2.3
1	A	291	THR	2.3
1	A	358	THR	2.3
1	D	242	LEU	2.3
1	D	254	SER	2.3
1	D	559	SER	2.3
1	K	435	SER	2.3
1	F	292	TYR	2.3
1	A	477	GLY	2.3
1	B	456	GLY	2.3
1	D	266	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	88	VAL	2.3
1	A	521	ASN	2.3
1	D	100	PRO	2.3
1	E	397	LYS	2.3
1	G	326	LYS	2.3
1	H	397	LYS	2.3
1	I	221	LYS	2.3
1	L	143	LYS	2.3
1	L	399	ASP	2.3
1	G	96	PRO	2.3
1	I	351	PRO	2.3
1	B	172	SER	2.3
1	D	460	ALA	2.3
1	E	93	SER	2.3
1	E	271	ILE	2.3
1	F	556	ILE	2.3
1	H	453	ILE	2.3
1	J	438	SER	2.3
1	C	452	THR	2.2
1	D	458	THR	2.2
1	F	239	LEU	2.2
1	G	509	LEU	2.2
1	A	262	GLU	2.2
1	B	125	GLU	2.2
1	E	578	GLY	2.2
1	H	532	GLU	2.2
1	H	586	ARG	2.2
1	J	594	ARG	2.2
1	K	200	GLU	2.2
1	L	381	GLY	2.2
1	J	480	TYR	2.2
1	A	278	LYS	2.2
1	D	303	ASN	2.2
1	D	394	ASP	2.2
1	D	582	ASN	2.2
1	F	397	LYS	2.2
1	G	265	LYS	2.2
1	I	181	ASN	2.2
1	I	457	ASN	2.2
1	L	386	LYS	2.2
1	C	561	PHE	2.2
1	E	503	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	523	PRO	2.2
1	B	124	GLU	2.2
1	E	380	SER	2.2
1	G	454	GLU	2.2
1	H	494	SER	2.2
1	B	488	THR	2.2
1	C	251	ARG	2.2
1	D	314	ALA	2.2
1	E	465	THR	2.2
1	F	248	THR	2.2
1	L	569	THR	2.2
1	E	336	LEU	2.2
1	G	346	LYS	2.2
1	H	589	LYS	2.2
1	I	353	LYS	2.2
1	E	176	TYR	2.2
1	I	538	ASN	2.2
1	L	457	ASN	2.2
1	C	319	GLN	2.2
1	C	532	GLU	2.2
1	D	89	PRO	2.2
1	D	307	PRO	2.2
1	F	406	VAL	2.2
1	H	296	GLN	2.2
1	I	334	GLU	2.2
1	E	236	ARG	2.2
1	J	199	SER	2.2
1	A	326	LYS	2.2
1	A	597	THR	2.2
1	C	329	GLY	2.2
1	C	347	GLY	2.2
1	C	469	ALA	2.2
1	C	477	GLY	2.2
1	I	373	GLY	2.2
1	J	490	ALA	2.2
1	E	322	ASN	2.2
1	E	333	LEU	2.2
1	G	352	ASN	2.2
1	I	483	ASP	2.2
1	K	575	ASP	2.2
1	K	177	MET	2.2
1	A	240	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	341	TYR	2.2
1	G	189	TYR	2.2
1	H	325	TYR	2.2
1	K	316	GLU	2.2
1	C	534	ARG	2.2
1	I	236	ARG	2.2
1	A	566	VAL	2.2
1	C	91	VAL	2.2
1	D	330	VAL	2.2
1	G	478	VAL	2.2
1	I	118	LYS	2.2
1	J	374	LYS	2.2
1	D	237	PHE	2.2
1	F	425	PHE	2.2
1	I	156	PHE	2.2
1	I	517	SER	2.2
1	H	373	GLY	2.2
1	J	375	GLY	2.2
1	C	340	ALA	2.2
1	D	543	ASP	2.2
1	G	212	THR	2.2
1	J	249	ASP	2.2
1	A	506	ASN	2.2
1	A	510	ILE	2.2
1	K	358	THR	2.2
1	L	415	THR	2.2
1	J	215	HIS	2.2
1	D	416	LEU	2.2
1	E	152	GLN	2.2
1	H	349	MET	2.2
1	J	111	LYS	2.2
1	J	118	LYS	2.2
1	K	360	LYS	2.2
1	L	353	LYS	2.2
1	A	418	PRO	2.2
1	B	288	TYR	2.2
1	J	141	PRO	2.2
1	E	269	VAL	2.2
1	G	206	VAL	2.2
1	H	516	SER	2.2
1	I	455	VAL	2.2
1	J	281	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	243	PHE	2.2
1	C	268	GLY	2.2
1	D	382	GLY	2.2
1	E	347	GLY	2.2
1	H	381	GLY	2.2
1	J	425	PHE	2.2
1	K	109	ASP	2.2
1	B	139	ASN	2.2
1	G	536	THR	2.2
1	H	108	HIS	2.2
1	H	186	ALA	2.2
1	J	166	ASN	2.2
1	A	105	THR	2.2
1	L	223	THR	2.2
1	L	314	ALA	2.2
1	C	327	ILE	2.2
1	A	265	LYS	2.2
1	D	589	LYS	2.2
1	E	168	LYS	2.2
1	H	168	LYS	2.2
1	L	338	MET	2.2
1	A	539	SER	2.2
1	C	154	SER	2.2
1	C	539	SER	2.2
1	F	246	TYR	2.2
1	F	343	SER	2.2
1	G	209	SER	2.2
1	G	245	GLU	2.2
1	I	555	SER	2.2
1	J	520	SER	2.2
1	A	150	ASP	2.2
1	A	381	GLY	2.2
1	B	347	GLY	2.2
1	E	249	ASP	2.2
1	K	287	TYR	2.2
1	F	290	GLY	2.2
1	E	568	ASN	2.2
1	F	132	VAL	2.2
1	F	217	ASN	2.2
1	K	566	VAL	2.2
1	F	354	PHE	2.2
1	G	235	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	367	LYS	2.2
1	B	589	LYS	2.2
1	C	186	ALA	2.2
1	E	232	LYS	2.2
1	E	253	LYS	2.2
1	E	337	LYS	2.2
1	D	241	THR	2.2
1	D	469	ALA	2.2
1	H	356	HIS	2.2
1	H	388	ALA	2.2
1	H	490	ALA	2.2
1	J	356	HIS	2.2
1	J	446	THR	2.2
1	B	453	ILE	2.2
1	E	264	ILE	2.2
1	F	327	ILE	2.2
1	C	227	GLU	2.2
1	G	262	GLU	2.2
1	K	135	PRO	2.2
1	L	389	PRO	2.2
1	D	216	ASP	2.2
1	F	517	SER	2.2
1	I	548	SER	2.2
1	B	563	LYS	2.1
1	F	137	LYS	2.1
1	F	386	LYS	2.1
1	H	367	LYS	2.1
1	I	126	GLY	2.2
1	I	545	ASN	2.1
1	K	149	ASN	2.1
1	L	320	LYS	2.1
1	C	359	TYR	2.1
1	A	153	VAL	2.1
1	D	534	ARG	2.1
1	J	583	PHE	2.1
1	K	573	HIS	2.1
1	C	284	ALA	2.1
1	C	535	ALA	2.1
1	F	358	THR	2.1
1	G	340	ALA	2.1
1	C	87	GLU	2.1
1	F	332	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	K	245	GLU	2.1
1	J	169	LEU	2.1
1	K	234	LEU	2.1
1	A	204	LYS	2.1
1	E	494	SER	2.1
1	H	389	PRO	2.1
1	J	302	SER	2.1
1	K	498	SER	2.1
1	L	346	LYS	2.1
1	L	438	SER	2.1
1	E	122	ASN	2.1
1	I	188	GLY	2.1
1	I	442	GLY	2.1
1	A	142	VAL	2.1
1	H	502	VAL	2.1
1	J	102	GLU	2.1
1	J	431	GLU	2.1
1	A	388	ALA	2.1
1	D	238	PHE	2.1
1	D	276	THR	2.1
1	E	519	THR	2.1
1	E	535	ALA	2.1
1	H	572	ALA	2.1
1	B	346	LYS	2.1
1	L	326	LYS	2.1
1	C	152	GLN	2.1
1	D	327	ILE	2.1
1	D	423	ILE	2.1
1	D	567	GLN	2.1
1	J	129	ILE	2.1
1	J	264	ILE	2.1
1	C	254	SER	2.1
1	C	548	SER	2.1
1	E	141	PRO	2.1
1	D	501	GLY	2.1
1	E	193	GLY	2.1
1	F	440	ARG	2.1
1	J	504	GLY	2.1
1	E	316	GLU	2.1
1	E	508	GLU	2.1
1	H	334	GLU	2.1
1	I	245	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	460	ALA	2.1
1	C	164	LYS	2.1
1	D	579	VAL	2.1
1	F	206	VAL	2.1
1	H	204	LYS	2.1
1	J	482	VAL	2.1
1	K	151	LYS	2.1
1	C	459	ASP	2.1
1	I	468	ASP	2.1
1	I	448	SER	2.1
1	K	146	SER	2.1
1	K	303	ASN	2.1
1	L	352	ASN	2.1
1	B	351	PRO	2.1
1	C	592	GLY	2.1
1	D	347	GLY	2.1
1	F	588	PRO	2.1
1	L	334	GLU	2.1
1	L	427	SER	2.1
1	J	317	LEU	2.1
1	J	336	LEU	2.1
1	K	94	LEU	2.1
1	L	450	GLY	2.1
1	E	247	MET	2.1
1	G	147	LYS	2.1
1	H	346	LYS	2.1
1	K	108	HIS	2.1
1	K	218	LYS	2.1
1	C	526	TRP	2.1
1	B	546	GLN	2.1
1	D	152	GLN	2.1
1	A	585	ALA	2.1
1	C	103	TYR	2.1
1	C	490	ALA	2.1
1	H	553	ALA	2.1
1	K	471	VAL	2.1
1	A	181	ASN	2.1
1	A	419	GLU	2.1
1	C	334	GLU	2.1
1	D	431	GLU	2.1
1	E	156	PHE	2.1
1	I	312	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	L	454	GLU	2.1
1	C	172	SER	2.1
1	I	119	GLY	2.1
1	J	191	GLY	2.1
1	H	529	ILE	2.1
1	C	253	LYS	2.1
1	E	416	LEU	2.1
1	F	234	LEU	2.1
1	H	368	LYS	2.1
1	J	210	LEU	2.1
1	J	253	LYS	2.1
1	D	424	HIS	2.1
1	E	479	ASP	2.1
1	K	443	ASP	2.1
1	D	415	THR	2.1
1	D	594	ARG	2.1
1	E	522	GLU	2.1
1	G	564	GLU	2.1
1	A	428	ALA	2.1
1	C	525	TRP	2.1
1	H	458	THR	2.1
1	J	586	ARG	2.1
1	L	171	THR	2.1
1	L	291	THR	2.1
1	K	437	ASN	2.1
1	K	521	ASN	2.1
1	L	299	ALA	2.1
1	A	92	VAL	2.1
1	D	344	VAL	2.1
1	D	478	VAL	2.1
1	E	211	VAL	2.1
1	B	325	TYR	2.1
1	B	359	TYR	2.1
1	E	417	LYS	2.1
1	G	311	SER	2.1
1	G	414	GLY	2.1
1	H	345	GLY	2.1
1	K	164	LYS	2.1
1	D	117	ILE	2.1
1	B	332	GLU	2.1
1	J	459	ASP	2.1
1	K	479	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	338	MET	2.1
1	L	236	ARG	2.1
1	E	366	LYS	2.1
1	F	212	THR	2.1
1	J	602	ASN	2.1
1	A	447	ALA	2.1
1	F	331	LYS	2.1
1	F	552	LYS	2.1
1	K	415	THR	2.1
1	I	428	ALA	2.1
1	D	295	SER	2.1
1	D	375	GLY	2.1
1	F	172	SER	2.1
1	H	193	GLY	2.1
1	L	539	SER	2.1
1	L	522	GLU	2.0
1	D	174	HIS	2.0
1	G	356	HIS	2.0
1	I	174	HIS	2.0
1	D	169	LEU	2.0
1	K	251	ARG	2.0
1	A	261	MET	2.0
1	B	540	LYS	2.0
1	J	518	LYS	2.0
1	L	563	LYS	2.0
1	H	183	ASN	2.0
1	F	171	THR	2.0
1	B	290	GLY	2.0
1	C	460	ALA	2.0
1	E	146	SER	2.0
1	E	191	GLY	2.0
1	F	456	GLY	2.0
1	G	126	GLY	2.0
1	H	578	GLY	2.0
1	J	578	GLY	2.0
1	L	489	GLY	2.0
1	F	324	GLU	2.0
1	J	324	GLU	2.0
1	A	89	PRO	2.0
1	C	478	VAL	2.0
1	E	88	VAL	2.0
1	J	113	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	I	189	TYR	2.0
1	J	287	TYR	2.0
1	E	221	LYS	2.0
1	K	423	ILE	2.0
1	C	212	THR	2.0
1	E	223	THR	2.0
1	J	456	GLY	2.0
1	A	380	SER	2.0
1	D	498	SER	2.0
1	E	469	ALA	2.0
1	H	500	ALA	2.0
1	D	399	ASP	2.0
1	A	173	LYS	2.0
1	C	224	VAL	2.0
1	D	269	VAL	2.0
1	G	91	VAL	2.0
1	G	471	VAL	2.0
1	J	540	LYS	2.0
1	K	111	LYS	2.0
1	H	215	HIS	2.0
1	L	114	VAL	2.0
1	A	565	PHE	2.0
1	A	161	ASN	2.0
1	E	134	ASN	2.0
1	F	383	TYR	2.0
1	H	457	ASN	2.0
1	K	506	ASN	2.0
1	L	246	TYR	2.0
1	A	250	GLU	2.0
1	G	324	GLU	2.0
1	G	431	GLU	2.0
1	B	339	GLY	2.0
1	C	113	GLN	2.0
1	D	177	MET	2.0
1	K	477	GLY	2.0
1	B	309	SER	2.0
1	B	468	ASP	2.0
1	C	331	LYS	2.0
1	E	443	ASP	2.0
1	E	458	THR	2.0
1	F	164	LYS	2.0
1	G	360	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	G	516	SER	2.0
1	H	97	THR	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
7	SO4	C	711	5/5	0.31	1.44	19.87	41,45,53,55	0
7	SO4	F	707	5/5	0.39	0.82	9.81	55,57,61,75	0
5	1PE	B	705	10/16	0.32	0.68	9.54	36,40,51,51	0
7	SO4	C	710	5/5	0.71	0.84	8.50	34,38,58,62	0
7	SO4	A	711	5/5	0.22	0.70	7.84	56,56,63,81	0
5	1PE	L	705	7/16	0.45	0.87	7.08	30,34,39,41	0
5	1PE	H	706	10/16	0.54	0.60	6.12	30,40,46,47	0
2	CO3	D	701	4/4	0.75	0.58	5.92	16,17,18,18	0
7	SO4	E	709	5/5	0.50	0.45	4.50	47,51,64,76	0
7	SO4	C	708	5/5	-0.03	0.66	4.48	53,57,64,72	0
2	CO3	K	701	4/4	0.68	0.51	4.17	19,19,19,21	0
2	CO3	E	701	4/4	0.83	0.48	3.90	16,18,18,21	0
7	SO4	A	712	5/5	0.73	0.63	3.59	36,42,50,54	0
7	SO4	G	711	5/5	0.52	0.62	3.34	46,48,51,55	0
5	1PE	D	706	10/16	0.60	0.46	3.22	27,36,40,41	0
5	1PE	K	706	12/16	0.48	0.38	2.94	26,36,43,48	0
7	SO4	K	708	5/5	0.21	0.52	2.94	58,60,74,75	0
2	CO3	J	701	4/4	0.80	0.47	2.70	15,16,17,20	0
5	1PE	I	706	11/16	0.46	0.41	2.16	26,35,48,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	1PE	A	705	9/16	0.63	0.54	2.13	25,32,36,39	0
5	1PE	J	707	10/16	0.46	0.44	1.92	27,34,42,52	0
2	CO3	I	701	4/4	0.87	0.38	1.91	15,15,16,17	0
4	4ZN	D	704	20/20	0.55	0.43	1.86	13,20,27,31	3
5	1PE	G	705	9/16	0.49	0.52	1.67	25,32,39,40	0
5	1PE	G	706	6/16	0.69	0.42	1.64	34,37,41,42	0
4	4ZN	B	704	16/20	0.55	0.43	1.55	11,19,24,31	3
5	1PE	G	707	6/16	0.49	0.47	1.54	31,35,39,39	0
5	1PE	C	706	9/16	0.67	0.34	1.35	26,29,35,36	0
5	1PE	F	705	10/16	0.40	0.39	1.19	26,37,45,52	0
5	1PE	L	706	10/16	0.65	0.39	1.17	31,38,45,48	0
5	1PE	J	705	11/16	0.25	0.44	1.15	33,40,50,52	0
5	1PE	E	706	12/16	0.53	0.38	0.96	25,33,43,44	0
4	4ZN	F	704	16/20	0.52	0.42	0.93	17,21,27,31	3
4	4ZN	G	704	16/20	0.51	0.44	0.92	14,17,22,23	4
4	4ZN	E	704	20/20	0.70	0.42	0.87	16,20,27,28	7
4	4ZN	L	704	16/20	0.53	0.44	0.86	14,18,23,27	3
2	CO3	C	701	4/4	0.52	0.40	0.78	15,16,18,18	0
4	4ZN	H	704	16/20	0.69	0.41	0.71	12,18,28,32	3
4	4ZN	C	704	16/20	0.69	0.37	0.62	15,18,23,24	4
4	4ZN	K	704	14/20	0.56	0.39	0.54	14,20,28,33	0
7	SO4	E	707	5/5	0.91	0.36	0.34	21,21,23,24	0
4	4ZN	I	704	12/20	0.70	0.34	0.25	16,18,22,23	0
2	CO3	B	701	4/4	0.74	0.33	0.18	16,16,16,20	0
2	CO3	L	701	4/4	0.60	0.38	0.14	16,17,18,19	0
7	SO4	G	709	5/5	0.92	0.33	-0.02	16,19,20,22	0
7	SO4	A	708	5/5	0.61	0.40	-0.03	44,47,50,58	0
4	4ZN	A	704	16/20	0.60	0.37	-0.12	15,17,22,23	3
7	SO4	J	708	5/5	0.95	0.29	-0.15	21,22,24,25	0
7	SO4	A	709	5/5	0.73	0.36	-0.17	53,57,75,78	0
2	CO3	H	701	4/4	0.67	0.34	-0.19	15,16,17,19	0
4	4ZN	J	704	16/20	0.72	0.30	-0.37	14,17,21,27	3
7	SO4	I	708	5/5	0.68	0.29	-0.57	74,74,83,91	0
2	CO3	G	701	4/4	0.62	0.33	-0.61	13,14,17,19	0
7	SO4	A	710	5/5	0.73	0.33	-0.62	36,40,54,59	0
2	CO3	F	701	4/4	0.56	0.31	-0.67	19,19,19,20	0
7	SO4	B	707	5/5	0.93	0.24	-1.11	17,19,23,24	0
2	CO3	A	701	4/4	0.72	0.29	-1.64	15,18,19,20	0
3	ZN	L	702	1/1	0.61	0.22	-1.68	18,18,18,18	0
7	SO4	G	710	5/5	0.75	0.21	-2.11	35,43,55,58	0
3	ZN	I	702	1/1	0.22	0.14	-2.56	19,19,19,19	0
3	ZN	C	702	1/1	0.54	0.17	-2.62	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	ZN	B	703	1/1	0.90	0.08	-3.16	15,15,15,15	0
3	ZN	K	703	1/1	0.92	0.14	-3.18	16,16,16,16	0
3	ZN	H	703	1/1	0.69	0.10	-3.25	15,15,15,15	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	-3.31	17,17,17,17	0
3	ZN	F	702	1/1	0.58	0.14	-3.46	22,22,22,22	0
3	ZN	K	702	1/1	0.91	0.08	-3.55	19,19,19,19	0
3	ZN	J	703	1/1	0.72	0.10	-3.63	15,15,15,15	0
3	ZN	H	702	1/1	0.74	0.08	-3.82	17,17,17,17	0
3	ZN	B	702	1/1	0.87	0.06	-3.84	17,17,17,17	0
3	ZN	D	703	1/1	0.82	0.10	-4.12	17,17,17,17	0
3	ZN	I	703	1/1	0.61	0.07	-4.42	19,19,19,19	0
3	ZN	G	702	1/1	0.70	0.10	-4.65	18,18,18,18	0
3	ZN	G	703	1/1	0.82	0.09	-4.76	15,15,15,15	0
3	ZN	E	702	1/1	0.96	0.07	-4.85	17,17,17,17	0
3	ZN	J	702	1/1	0.71	0.09	-4.97	19,19,19,19	0
3	ZN	F	703	1/1	0.97	0.08	-4.98	18,18,18,18	0
3	ZN	A	703	1/1	0.82	0.10	-5.10	14,14,14,14	0
3	ZN	A	702	1/1	0.67	0.16	-5.43	18,18,18,18	0
3	ZN	D	702	1/1	0.73	0.11	-6.28	17,17,17,17	0
3	ZN	E	703	1/1	0.73	0.08	-10.11	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	0.34	0.59	-	55,55,63,82	0
5	1PE	K	705	12/16	0.37	0.37	-	29,41,46,47	0
5	1PE	A	706	12/16	-0.04	0.89	-	33,46,50,51	0
7	SO4	G	708	5/5	0.85	0.33	-	41,43,46,58	0
7	SO4	J	709	5/5	0.56	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	0.53	0.47	-	57,57,57,58	0
5	1PE	D	705	10/16	0.01	0.52	-	27,37,45,48	0
7	SO4	L	707	5/5	0.80	0.39	-	62,63,64,66	0
5	1PE	I	705	12/16	0.53	0.30	-	35,40,43,47	0
5	1PE	C	705	13/16	0.41	0.35	-	27,41,52,52	0
5	1PE	B	706	10/16	0.47	0.57	-	41,45,54,56	0
7	SO4	D	707	5/5	0.74	0.36	-	42,43,57,58	0
7	SO4	F	706	5/5	0.86	0.40	-	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	0.45	-	29,39,44,45	0
6	GOL	A	707	6/6	0.27	0.58	-	37,37,45,54	0
5	1PE	H	705	10/16	0.36	0.62	-	35,44,50,53	0
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.