



# Full wwPDB X-ray Structure Validation Report

(i)

Feb 27, 2014 – 12:50 PM GMT

PDB ID : 3DL8

Title : Structure of the complex of aquifex aeolicus SecYEG and bacillus subtilis SecA

Authors : Nam, Y.; Zimmer, J.; Rapoport, T.A.

Deposited on : 2008-06-26

Resolution : 7.50 Å (reported)

This is a full wwPDB validation report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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

MolProbity : 4.02b-467

Mogul : 1.15 2013

Xtriage (Phenix) : dev-1323

EDS : stable22639

Percentile statistics : 21963

Refmac : 5.8.0049

CCP4 : 6.3.0 (Settle)

Ideal geometry (proteins) : Engh & Huber (2001)

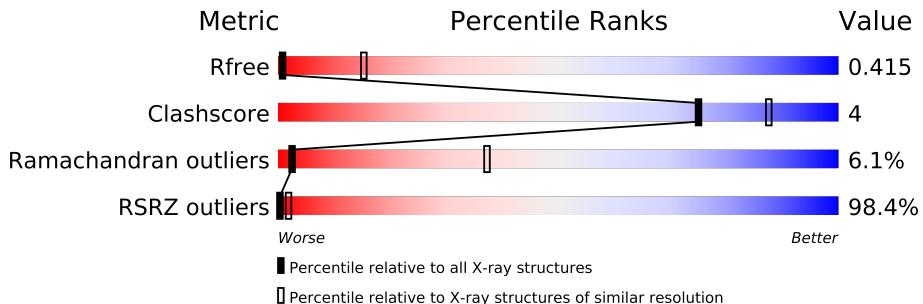
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)

Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance (i)

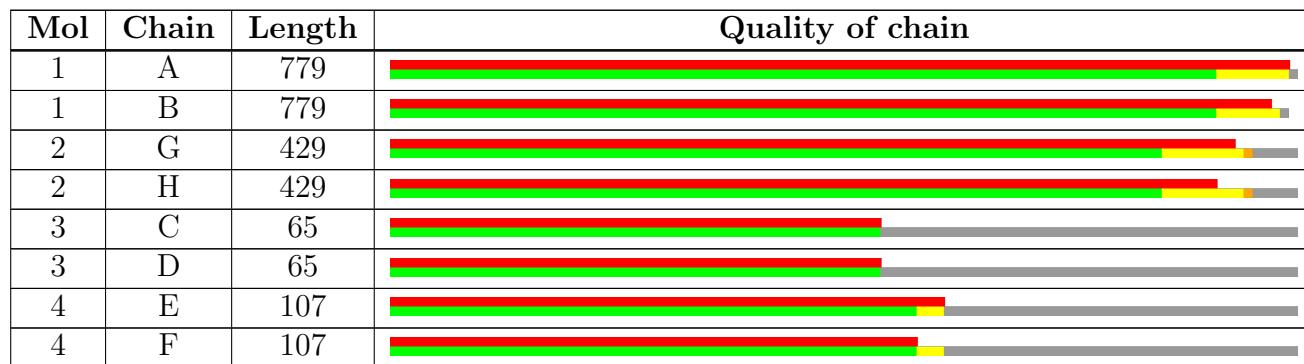
The reported resolution of this entry is 7.50 Å.

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))
$R_{free}$	66092	1106 (11.50-3.50)
Clashscore	79885	1039 (10.00-3.52)
Ramachandran outliers	78287	1301 (11.50-3.50)
RSRZ outliers	66119	1105 (11.50-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.



## 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10232 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Protein translocase subunit secA.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
1	A	773	Total C	N	O	0	0	0
			3092 1546	773	773			

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
1	B	773	Total C	N	O	0	0	0
			3092 1546	773	773			

- Molecule 2 is a protein called Preprotein translocase subunit secY.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	G	406	Total C	N	O	0	0	0
			1624 812	406	406			

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	H	406	Total C	N	O	0	0	0
			1624 812	406	406			

- Molecule 3 is a protein called SecE.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	C	35	Total C	N	O	0	0	0
			140 70	35	35			

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	D	35	Total C	N	O	0	0	0
			140 70	35	35			

- Molecule 4 is a protein called Protein-export membrane protein secG.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	E	65	Total C	N	O	0	0	0
			260 130	65	65			

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	F	65	Total C	N	O	0	0	0
			260 130	65	65			

There are 14 discrepancies between the modelled and reference sequences:

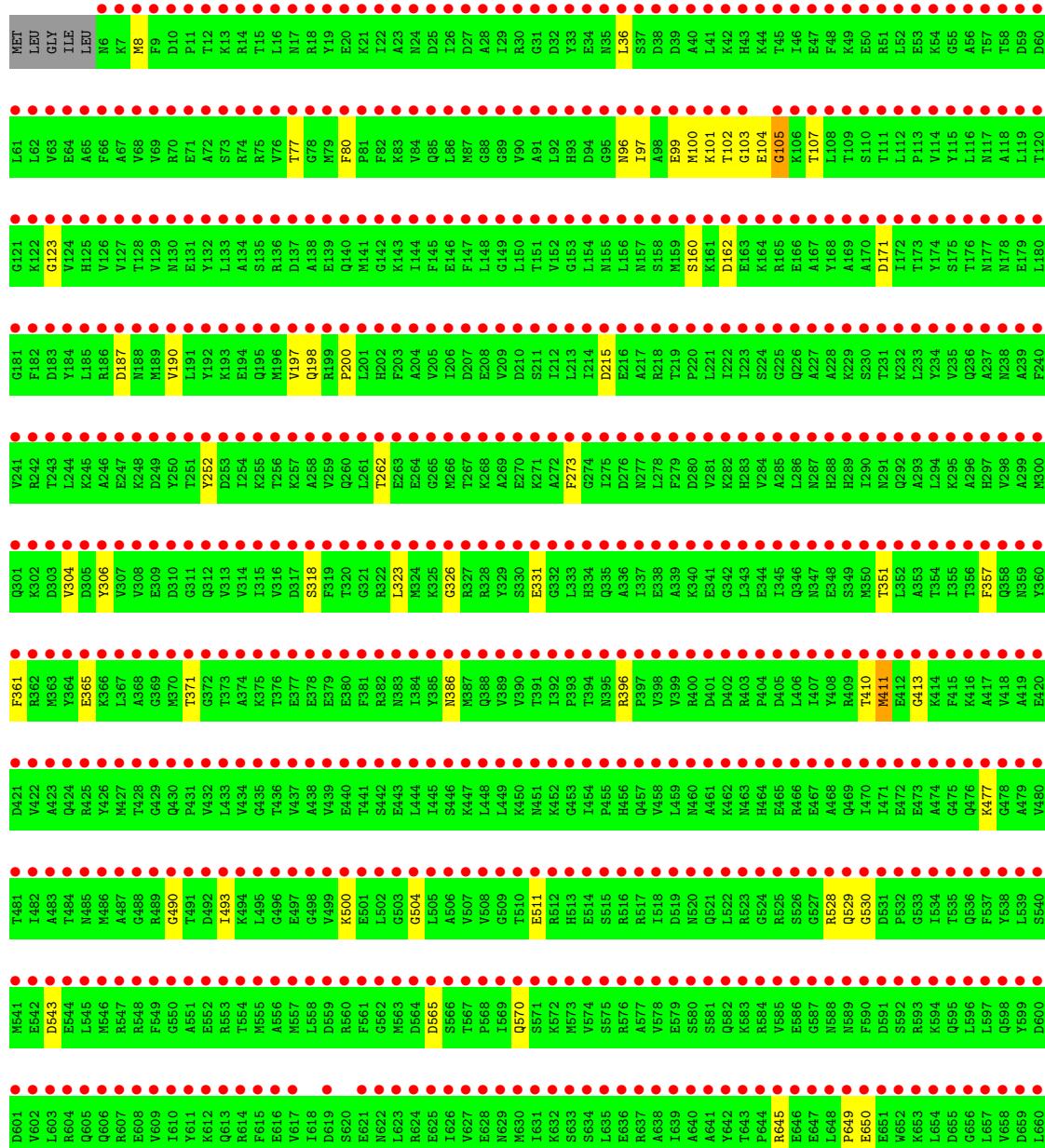
Chain	Residue	Modelled	Actual	Comment	Reference
E	101	GLY	-	EXPRESSION TAG	UNP O66505
E	102	HIS	-	EXPRESSION TAG	UNP O66505
E	103	HIS	-	INSERTION	UNP O66505
E	104	HIS	-	EXPRESSION TAG	UNP O66505
E	105	HIS	-	EXPRESSION TAG	UNP O66505
E	106	HIS	-	EXPRESSION TAG	UNP O66505
E	107	HIS	-	EXPRESSION TAG	UNP O66505
F	101	GLY	-	EXPRESSION TAG	UNP O66505
F	102	HIS	-	EXPRESSION TAG	UNP O66505
F	103	HIS	-	EXPRESSION TAG	UNP O66505
F	104	HIS	-	EXPRESSION TAG	UNP O66505
F	105	HIS	-	EXPRESSION TAG	UNP O66505
F	106	HIS	-	EXPRESSION TAG	UNP O66505
F	107	HIS	-	EXPRESSION TAG	UNP O66505

### 3 Residue-property plots

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

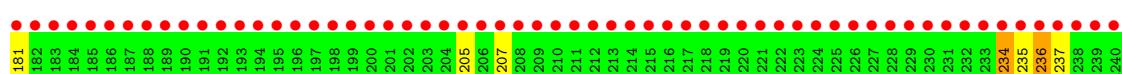
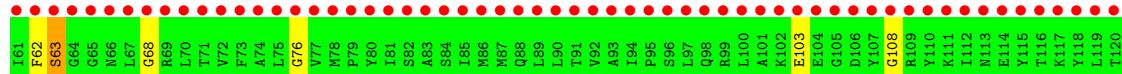
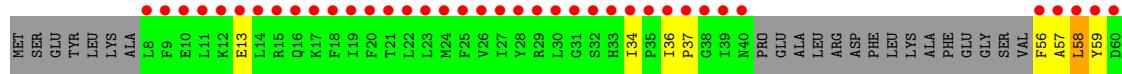
Chain A: 



T664	L603	D543	A423	Q301	G181	G121	D721	I681
Y665	R604	E544	Q424	K302	R242	S722	N662	N661
L666	R605	L545	N425	X303	T243	K723	T663	T663
Q606	R607	R547	M426	M304	E244	V724	W724	T664
D667	E668	E548	R428	R305	M366	L124	D726	Y665
C669	E608	R549	G429	Y306	A246	R125	H725	F666
A670	R609	F649	G430	V307	E247	V126	H727	K77
L671	I610	G550	P430	M570	E248	V127	H728	M68
E672	Y611	A551	P431	T371	E309	D249	D729	T668
K673	R612	E552	D432	V372	D310	Y250	A730	E774
R674	Q613	R553	I433	T373	D312	L190	R70	I576
D675	R614	T554	K494	A374	A374	L185	E71	F677
I676	F615	M555	L435	G375	A366	R126	A712	G578
F677	E616	A556	G496	K376	V308	V127	D732	H737
G678	V617	M557	E497	V377	D377	K255	V128	K773
K679	R618	L558	A438	E378	S318	K256	A733	S374
E680	D619	D559	V499	V379	F319	V190	D734	D775
P681	S620	R560	K500	E430	T320	L191	A735	T676
D682	E621	E561	E501	T441	F381	V192	R711	F677
E683	N622	G562	L502	R442	N382	V259	H739	K679
M684	L623	M563	G503	E443	N383	E194	R740	E774
I685	R624	D564	G504	I444	T384	M195	V741	P881
E686	L625	S565	V499	V379	E379	T256	A742	D881
L687	T626	S566	K505	E445	V385	M196	R743	Q736
I688	V627	T567	V507	K446	N386	V197	A744	F777
M689	E628	P568	M508	I447	N387	K257	R745	G778
D690	N629	I569	G509	A448	Q388	V258	V746	H779
R691	M630	Q570	T540	K450	V390	S330	E200	E779
E692	L631	E571	E511	N451	T391	K326	F203	T677
K693	K632	K572	R512	K452	I392	E264	A204	A777
T694	S633	H513	C453	A453	P393	L333	V205	R746
I695	S334	E574	E514	I454	T394	H334	E206	V747
Y696	S635	S575	S515	P455	M395	H335	D207	D748
N697	E636	R576	R516	H456	R396	A336	V208	P749
E698	R637	A577	R517	V457	P397	I337	E209	Y749
K699	A638	V578	T518	V458	V398	E338	D210	M689
E700	I639	E579	D519	I459	V399	A339	V210	R690
E701	A640	S580	N520	E460	P400	A340	E211	E755
Q702	A641	S581	Q521	A461	D401	E341	V212	R691
F703	Y642	Q582	L522	K462	D402	G342	E213	E756
R709	T643	K583	R523	N463	R403	E343	V214	V757
K705	P644	R584	G524	H464	P404	E344	K222	E758
E706	B645	V585	H525	E465	D405	T345	V223	D762
E707	E546	E586	S526	E466	A406	Q346	S224	F703
M708	Q587	G587	G527	E467	A407	N347	G225	R709
P649	N588	Q588	Q528	A468	R408	E348	E226	D763
E650	N589	Q529	Q529	Q469	R409	S349	A227	E770
F711	E651	E651	E651	J470	T410	M360	K102	E771
E712	D652	D591	D531	I471	E411	E162	K102	D764
E706	P552	P532	P532	E472	E412	E163	G103	R709
Q707	E546	E586	E586	E473	E413	E164	E104	E772
E708	E546	E586	E586	E474	E414	E165	R511	E773
R709	P649	P649	P649	E475	E415	E166	L512	E774
F710	E651	E651	E651	J470	T410	M360	K102	E775
F711	D652	D591	D531	I471	E411	E162	G103	D765
E712	P552	P532	P532	E472	E412	E163	E104	R709
K713	K653	K593	K593	E473	E413	E164	E104	E776
V714	L654	I594	I594	E474	E414	E165	R511	E777
T715	I715	D655	D655	E475	E415	E166	L512	E778
L716	G656	Q595	Q595	J470	T410	M360	K102	E779
R717	L657	L595	L595	I471	E411	E162	G103	D766
V718	W658	W598	W598	E472	E412	E163	E104	R709
A719	D659	Y598	Y598	E473	E413	E164	E104	E777
V720	L660	Y599	Y599	E474	E414	E165	R511	E778
D721	I661	S540	S540	V480	E420	E166	L512	R718
S722	N662	D601	N662	T481	D421	E167	E105	A779
K723	V663	E542	E542	V482	R422	E168	D601	C7U

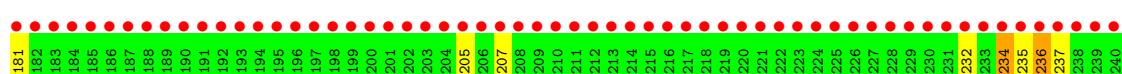
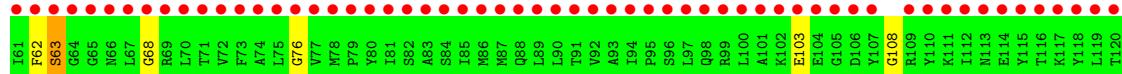
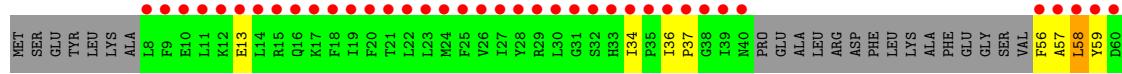
- Molecule 2: Preprotein translocase subunit secY

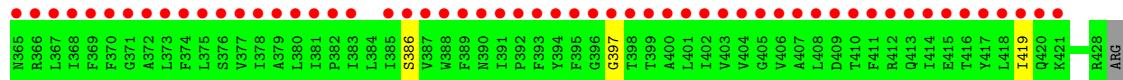
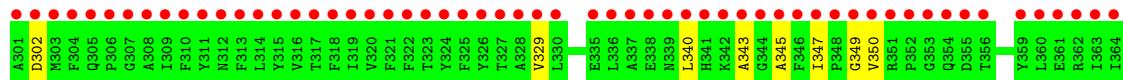
Chain G:



- Molecule 2: Preprotein translocase subunit secY

### Chain H:





- Molecule 3: SecE

Chain C:



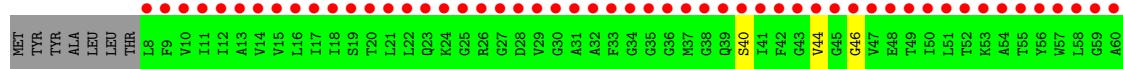
- Molecule 3: SecE

Chain D:



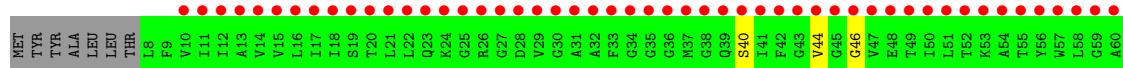
- Molecule 4: Protein-export membrane protein secG

Chain E:



- Molecule 4: Protein-export membrane protein secG

Chain F:



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	146.36 Å    167.97 Å    187.72 Å 90.00°    90.00°    90.00°	Depositor
Resolution (Å)	14.99 – 7.50 48.09 – 7.49	Depositor EDS
% Data completeness (in resolution range)	99.5 (14.99-7.50) 99.0 (48.09-7.49)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) >$ <sup>1</sup>	2.28 (at 7.37 Å)	Xtriage
Refinement program	CNS 1.2	Depositor
$R$ , $R_{free}$	0.365 , 0.390 0.411 , 0.415	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	530.1	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	28.97 , 207.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$<  L  > = 0.43$ , $< L^2 > = 0.26$	Xtriage
Outliers	1 of 6217 reflections (0.016%)	Xtriage
$F_o, F_c$ correlation	0.62	EDS
Total number of atoms	10232	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	452.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.91% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality (i)

### 5.1 Standard geometry (i)

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	0.88	0/3091	0.90	2/3862 (0.1%)
1	B	0.88	0/3091	0.90	2/3862 (0.1%)
2	G	0.98	0/1622	0.96	2/2024 (0.1%)
2	H	0.97	0/1622	0.96	2/2024 (0.1%)
3	C	0.94	0/139	0.75	0/172
3	D	0.94	0/139	0.75	0/172
4	E	1.02	0/259	0.93	0/322
4	F	1.02	0/259	0.93	0/322
All	All	0.92	0/10222	0.92	8/12760 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	160	SER	N-CA-C	-7.19	91.59	111.00
1	B	160	SER	N-CA-C	-7.17	91.63	111.00
1	A	304	VAL	C-N-CA	6.29	137.41	121.70
1	B	304	VAL	C-N-CA	6.25	137.31	121.70
2	H	302	ASP	C-N-CA	-5.36	108.31	121.70
2	G	235	VAL	C-N-CA	5.31	134.97	121.70
2	G	302	ASP	C-N-CA	-5.29	108.49	121.70
2	H	235	VAL	C-N-CA	5.26	134.85	121.70

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProBity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the

chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3092	0	856	18	0
1	B	3092	0	856	12	0
2	G	1624	0	446	17	0
2	H	1624	0	446	13	0
3	C	140	0	36	0	0
3	D	140	0	36	0	0
4	E	260	0	86	1	0
4	F	260	0	86	1	0
All	All	10232	0	2848	52	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (52) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:776:MET:O	1:B:778:ALA:O	1.54	1.25
1:A:776:MET:O	1:B:778:ALA:C	1.98	1.02
1:A:778:ALA:C	1:B:776:MET:O	1.99	1.00
1:A:778:ALA:O	1:B:776:MET:O	1.83	0.95
2:H:103:GLU:H	2:H:108:GLY:HA3	1.39	0.86
2:G:103:GLU:H	2:G:108:GLY:HA3	1.39	0.85
1:A:726:ASP:O	2:G:258:GLY:CA	2.29	0.80
1:A:726:ASP:O	2:G:258:GLY:HA2	1.84	0.77
2:H:103:GLU:H	2:H:108:GLY:CA	2.03	0.72
2:G:103:GLU:H	2:G:108:GLY:CA	2.03	0.71
1:A:726:ASP:C	2:G:258:GLY:HA2	2.16	0.64
1:A:726:ASP:O	2:G:258:GLY:HA3	2.00	0.62
2:H:57:ALA:O	2:H:59:TYR:N	2.33	0.62
2:G:57:ALA:O	2:G:59:TYR:N	2.33	0.61
1:B:103:GLY:H	1:B:529:GLN:H	1.47	0.61
2:H:56:PHE:O	2:H:63:SER:CA	2.48	0.61
2:G:56:PHE:O	2:G:63:SER:CA	2.48	0.60
1:A:103:GLY:H	1:A:529:GLN:H	1.47	0.59
2:G:56:PHE:O	2:G:63:SER:C	2.42	0.58
2:G:343:ALA:O	2:G:349:GLY:HA3	2.03	0.58
2:H:343:ALA:O	2:H:349:GLY:HA3	2.03	0.58
2:H:56:PHE:O	2:H:63:SER:C	2.42	0.57
1:A:500:LYS:CA	1:A:504:GLY:HA2	2.35	0.57
1:B:500:LYS:CA	1:B:504:GLY:HA2	2.35	0.56
2:H:57:ALA:O	2:H:58:LEU:C	2.46	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:G:57:ALA:O	2:G:58:LEU:C	2.46	0.52
1:B:103:GLY:N	1:B:529:GLN:H	2.09	0.51
1:A:778:ALA:CA	1:B:776:MET:O	2.59	0.50
1:A:103:GLY:N	1:A:529:GLN:H	2.09	0.50
1:A:331:GLU:N	2:G:253:ARG:O	2.35	0.49
2:H:103:GLU:N	2:H:108:GLY:HA3	2.20	0.47
1:B:123:GLY:HA2	1:B:171:ASP:O	2.14	0.47
1:A:123:GLY:HA2	1:A:171:ASP:O	2.14	0.47
2:G:103:GLU:N	2:G:108:GLY:HA3	2.20	0.47
4:E:44:VAL:C	4:E:46:GLY:H	2.20	0.45
1:A:411:MET:C	1:A:413:GLY:H	2.21	0.45
4:F:44:VAL:C	4:F:46:GLY:H	2.20	0.44
2:H:62:PHE:O	2:H:63:SER:O	2.35	0.44
2:G:62:PHE:O	2:G:63:SER:O	2.35	0.44
1:B:411:MET:C	1:B:413:GLY:H	2.21	0.44
2:H:161:THR:O	2:H:165:GLY:HA3	2.19	0.43
2:G:161:THR:O	2:G:165:GLY:HA3	2.19	0.43
1:A:105:GLY:O	1:A:107:THR:N	2.50	0.42
2:G:234:TYR:C	2:G:236:GLN:H	2.23	0.42
2:H:153:SER:C	2:H:155:ILE:N	2.72	0.42
1:A:528:ARG:C	1:A:530:GLY:H	2.24	0.41
1:B:105:GLY:O	1:B:107:THR:N	2.50	0.41
1:B:85:GLN:C	1:B:88:GLY:H	2.25	0.41
2:H:234:TYR:C	2:H:236:GLN:H	2.23	0.40
2:G:234:TYR:C	2:G:236:GLN:N	2.74	0.40
1:A:357:PHE:O	1:A:361:PHE:N	2.54	0.40
2:H:232:ILE:C	2:H:234:TYR:N	2.74	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	771/779 (99%)	638 (83%)	86 (11%)	47 (6%)	2   37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	771/779 (99%)	638 (83%)	85 (11%)	48 (6%)	2 37
2	G	402/429 (94%)	321 (80%)	52 (13%)	29 (7%)	2 32
2	H	402/429 (94%)	319 (79%)	54 (13%)	29 (7%)	2 32
3	C	33/65 (51%)	33 (100%)	0	0	100 100
3	D	33/65 (51%)	33 (100%)	0	0	100 100
4	E	63/107 (59%)	57 (90%)	5 (8%)	1 (2%)	14 71
4	F	63/107 (59%)	57 (90%)	5 (8%)	1 (2%)	14 71
All	All	2538/2760 (92%)	2096 (83%)	287 (11%)	155 (6%)	2 37

All (155) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	LEU
1	A	80	PHE
1	A	99	GLU
1	A	100	MET
1	A	101	LYS
1	A	197	VAL
1	A	306	TYR
1	A	326	GLY
1	A	371	THR
1	A	543	ASP
1	A	570	GLN
1	A	645	ARG
1	A	649	PRO
1	A	650	GLU
1	A	744	ALA
1	B	36	LEU
1	B	80	PHE
1	B	99	GLU
1	B	100	MET
1	B	101	LYS
1	B	197	VAL
1	B	306	TYR
1	B	326	GLY
1	B	371	THR
1	B	543	ASP
1	B	570	GLN
1	B	645	ARG
1	B	649	PRO

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Mol	Chain	Res	Type
1	B	650	GLU
1	B	744	ALA
2	G	36	ILE
2	G	37	PRO
2	G	58	LEU
2	G	63	SER
2	G	236	GLN
2	G	347	ILE
2	G	350	VAL
2	H	36	ILE
2	H	37	PRO
2	H	58	LEU
2	H	63	SER
2	H	236	GLN
2	H	347	ILE
2	H	350	VAL
1	A	8	MET
1	A	102	THR
1	A	104	GLU
1	A	198	GLN
1	A	252	TYR
1	A	351	THR
1	A	410	THR
1	A	477	LYS
1	A	490	GLY
1	A	676	ILE
1	B	8	MET
1	B	102	THR
1	B	104	GLU
1	B	198	GLN
1	B	252	TYR
1	B	351	THR
1	B	410	THR
1	B	477	LYS
1	B	490	GLY
1	B	676	ILE
2	G	181	ILE
2	G	237	GLU
2	G	257	ALA
2	G	340	LEU
2	G	419	ILE
2	H	181	ILE

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Mol	Chain	Res	Type
2	H	237	GLU
2	H	257	ALA
2	H	340	LEU
2	H	419	ILE
4	E	40	SER
4	F	40	SER
1	A	187	ASP
1	A	262	THR
1	A	323	LEU
1	A	493	ILE
1	A	511	GLU
1	A	565	ASP
1	A	678	GLY
1	B	187	ASP
1	B	262	THR
1	B	323	LEU
1	B	493	ILE
1	B	511	GLU
1	B	565	ASP
1	B	678	GLY
2	G	13	GLU
2	G	207	LYS
2	G	234	TYR
2	G	329	VAL
2	G	345	ALA
2	H	13	GLU
2	H	207	LYS
2	H	234	TYR
2	H	329	VAL
2	H	345	ALA
1	A	77	THR
1	A	96	ASN
1	A	162	ASP
1	A	273	PHE
1	A	365	GLU
1	A	386	ASN
1	A	745	GLN
1	B	77	THR
1	B	96	ASN
1	B	162	ASP
1	B	200	PRO
1	B	273	PHE

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Mol	Chain	Res	Type
1	B	365	GLU
1	B	386	ASN
1	B	745	GLN
2	G	150	PRO
2	G	153	SER
2	G	205	TYR
2	G	269	PRO
2	G	272	VAL
2	H	150	PRO
2	H	153	SER
2	H	205	TYR
2	H	269	PRO
2	H	272	VAL
1	A	200	PRO
1	A	318	SER
1	A	411	MET
1	B	318	SER
1	B	411	MET
2	G	76	GLY
2	G	141	PRO
2	G	243	PRO
2	G	386	SER
2	G	397	GLY
2	H	76	GLY
2	H	141	PRO
2	H	243	PRO
2	H	386	SER
2	H	397	GLY
1	A	105	GLY
1	A	215	ASP
1	B	105	GLY
1	B	171	ASP
1	B	215	ASP
2	G	68	GLY
2	H	68	GLY
1	A	97	ILE
1	A	396	ARG
1	B	97	ILE
1	B	396	ARG
1	A	190	VAL
1	B	190	VAL
2	G	34	ILE

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Mol	Chain	Res	Type
2	H	34	ILE

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

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

### 5.3.3 RNA [\(i\)](#)

There are no RNA chains in this entry.

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

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

### 5.5 Carbohydrates [\(i\)](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [\(i\)](#)

There are no ligands in this entry.

### 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data (i)

### 6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	773/779 (99%)	15.31	768 (99%) 0   1	321, 444, 550, 648	0
1	B	773/779 (99%)	13.48	759 (98%) 0   2	340, 470, 540, 612	0
2	G	406/429 (94%)	15.20	401 (98%) 0   2	321, 409, 488, 512	0
2	H	406/429 (94%)	13.36	391 (96%) 0   2	372, 466, 536, 558	0
3	C	35/65 (53%)	22.79	35 (100%) 0   1	328, 363, 402, 405	0
3	D	35/65 (53%)	26.15	35 (100%) 0   1	383, 396, 463, 466	0
4	E	65/107 (60%)	12.29	65 (100%) 0   1	386, 446, 468, 473	0
4	F	65/107 (60%)	10.72	62 (95%) 0   2	477, 523, 550, 551	0
All	All	2558/2760 (92%)	14.49	2516 (98%) 0   2	321, 450, 541, 648	0

All (2516) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	117	LYS	61.3
1	A	50	GLU	57.8
1	A	51	ARG	56.3
1	A	120	THR	54.6
2	G	121	LEU	54.4
1	A	558	LEU	53.8
2	G	363	ILE	53.4
1	A	562	GLY	53.2
2	G	362	ARG	52.8
1	B	467	GLU	51.2
1	B	765	GLU	49.2
1	A	47	GLU	49.1
2	G	311	TYR	48.4
1	A	282	LYS	48.3
1	A	430	GLN	46.7
1	A	44	LYS	46.3

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Mol	Chain	Res	Type	RSRZ
3	D	49	LEU	46.0
2	G	366	ARG	45.7
1	B	538	TYR	45.1
2	G	315	TYR	44.6
1	A	266	MET	44.5
1	B	768	GLU	44.3
1	A	281	VAL	44.3
1	B	555	MET	44.2
1	B	209	VAL	43.8
2	G	361	GLU	43.5
2	H	167	MET	43.3
1	A	536	GLN	42.9
3	D	50	THR	42.4
2	G	124	ALA	42.3
1	B	763	MET	42.0
1	A	52	LEU	41.6
1	A	53	GLU	41.4
1	A	45	THR	41.1
1	A	559	ASP	40.8
2	G	364	ILE	40.7
1	A	280	ASP	40.7
1	B	481	THR	40.6
1	A	264	GLU	40.5
1	B	534	ILE	40.2
1	B	30	ARG	40.2
1	A	174	TYR	40.0
1	A	538	TYR	40.0
3	D	39	ALA	39.1
1	A	534	ILE	39.1
3	D	42	VAL	39.0
1	A	535	THR	39.0
1	A	117	ASN	38.7
3	C	53	LYS	38.5
1	A	557	MET	38.4
2	G	342	LYS	38.4
2	H	290	ASN	38.2
2	H	33	HIS	38.1
2	H	350	VAL	37.9
2	G	354	GLN	37.7
1	A	54	LYS	37.7
2	G	120	THR	37.7
1	A	632	LYS	37.6

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Mol	Chain	Res	Type	RSRZ
1	A	701	GLU	37.6
2	H	217	THR	37.5
3	C	55	ILE	37.3
1	A	687	LEU	37.3
3	D	53	LYS	37.2
1	A	125	HIS	37.1
1	A	510	THR	36.8
1	B	764	ILE	36.7
3	D	31	ILE	36.5
2	G	352	PRO	36.4
1	B	31	GLY	36.3
1	A	478	GLY	36.1
1	B	269	ALA	36.1
1	A	267	THR	36.1
2	H	157	ILE	36.0
1	A	479	ALA	35.8
2	G	30	LEU	35.8
2	G	119	LEU	35.7
1	B	767	ILE	35.7
2	H	29	ARG	35.6
2	G	118	TYR	35.6
1	A	265	GLY	35.6
1	A	630	MET	35.6
2	G	322	PHE	35.6
1	B	554	THR	35.5
2	G	360	LEU	35.5
1	A	635	LEU	35.3
2	G	355	ASP	35.1
2	G	356	THR	35.1
2	H	30	LEU	34.9
1	A	537	PHE	34.8
2	G	314	LEU	34.7
2	G	132	ALA	34.6
1	A	638	ALA	34.6
2	H	216	LEU	34.5
1	B	557	MET	34.4
2	G	283	LEU	34.4
1	A	609	VAL	34.3
1	A	382	ARG	34.3
1	B	280	ASP	34.2
2	H	155	ILE	34.0
1	A	279	PHE	33.9

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Mol	Chain	Res	Type	RSRZ
4	F	60	ALA	33.8
1	A	212	ILE	33.8
1	A	628	GLU	33.5
1	A	445	ILE	33.5
1	B	769	ASP	33.5
1	A	232	LYS	33.5
2	G	341	HIS	33.5
1	B	566	SER	33.4
1	A	124	VAL	33.4
3	C	54	ILE	33.3
2	G	358	LYS	33.2
2	G	324	TYR	33.2
1	A	49	LYS	33.2
3	D	30	THR	33.1
1	B	270	GLU	33.1
2	G	317	THR	33.1
2	G	312	ASN	33.1
1	A	563	MET	33.1
1	A	48	PHE	33.0
1	A	173	THR	33.0
2	G	323	THR	32.8
1	A	639	ILE	32.7
2	G	316	VAL	32.7
2	H	215	PRO	32.7
3	D	33	VAL	32.7
1	A	483	ALA	32.5
2	G	27	ILE	32.4
2	G	198	PRO	32.4
1	B	470	ILE	32.3
1	A	435	GLY	32.3
2	H	28	TYR	32.3
3	D	36	PHE	32.3
2	G	115	TYR	32.3
1	B	62	LEU	32.2
1	B	718	ARG	32.2
1	B	265	GLY	32.1
2	G	135	ILE	32.0
2	G	29	ARG	32.0
1	B	475	GLY	31.9
2	H	372	ALA	31.8
1	A	509	GLY	31.8
2	H	176	ILE	31.7

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Mol	Chain	Res	Type	RSRZ
1	A	268	LYS	31.5
1	B	464	HIS	31.5
1	B	762	HIS	31.3
1	A	380	GLU	31.3
3	D	40	ILE	31.3
1	A	116	LEU	31.2
2	G	359	TYR	31.1
1	A	426	TYR	31.0
1	B	469	GLN	31.0
2	G	116	THR	31.0
1	B	532	PRO	30.9
1	B	382	ARG	30.9
1	A	625	GLU	30.9
1	B	471	ILE	30.8
1	B	565	ASP	30.8
2	H	218	LEU	30.8
2	G	313	PHE	30.7
1	B	719	ALA	30.7
1	A	46	ILE	30.7
1	A	560	ARG	30.6
2	H	158	THR	30.6
3	D	38	LEU	30.6
1	B	268	LYS	30.6
1	A	631	ILE	30.5
4	E	23	GLN	30.5
3	D	54	ILE	30.5
2	G	123	VAL	30.5
1	A	448	LEU	30.5
3	D	46	ILE	30.5
1	B	497	GLU	30.4
2	G	28	TYR	30.4
1	A	650	GLU	30.4
2	G	241	ARG	30.3
1	B	466	ARG	30.3
1	A	520	ASN	30.3
1	B	433	LEU	30.3
2	G	357	VAL	30.3
2	G	125	THR	30.2
1	A	522	LEU	30.2
1	B	266	MET	30.2
2	H	289	LEU	30.2
2	G	114	GLU	30.1

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Mol	Chain	Res	Type	RSRZ
1	A	762	HIS	30.1
4	F	20	THR	30.1
1	A	381	PHE	30.1
1	A	457	GLN	30.0
1	A	58	THR	30.0
2	H	166	THR	30.0
1	B	274	GLY	30.0
2	H	219	LEU	29.9
1	B	536	GLN	29.9
1	B	623	LEU	29.8
1	B	473	GLU	29.7
3	C	43	TYR	29.7
3	D	35	ILE	29.7
1	B	766	SER	29.7
2	G	122	PHE	29.6
1	A	431	PRO	29.6
1	B	474	ALA	29.5
1	A	441	THR	29.4
1	B	283	HIS	29.4
1	B	26	ILE	29.4
2	G	113	ASN	29.4
2	G	200	ALA	29.3
2	H	221	ILE	29.3
1	B	184	TYR	29.3
4	E	24	LYS	29.2
2	H	156	LEU	29.2
1	B	41	LEU	29.1
2	G	282	LEU	29.1
2	H	34	ILE	29.0
1	A	172	ILE	29.0
1	B	759	MET	29.0
1	B	476	GLN	28.9
1	B	499	VAL	28.9
3	D	43	TYR	28.9
2	G	281	LEU	28.8
3	D	41	GLY	28.8
2	H	315	TYR	28.8
1	B	457	GLN	28.8
2	G	350	VAL	28.7
1	A	320	THR	28.7
1	A	118	ALA	28.7
1	B	542	GLU	28.7

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Mol	Chain	Res	Type	RSRZ
1	B	281	VAL	28.6
1	B	539	LEU	28.6
1	A	539	LEU	28.6
1	A	283	HIS	28.6
2	G	203	GLN	28.5
1	B	761	GLU	28.5
1	A	629	ASN	28.5
2	H	288	LEU	28.4
1	B	567	THR	28.4
3	C	46	ILE	28.4
2	G	365	ASN	28.4
1	B	533	GLY	28.3
2	G	33	HIS	28.3
2	G	367	LEU	28.3
4	F	19	SER	28.3
1	B	556	ALA	28.3
2	H	160	LEU	28.3
1	A	402	ASP	28.2
1	B	385	TYR	28.2
1	A	436	THR	28.2
1	B	468	ALA	28.2
2	G	199	ASN	28.1
1	B	500	LYS	28.1
1	B	715	ILE	28.1
1	B	564	ASP	28.0
3	C	47	LEU	27.9
1	A	278	LEU	27.9
1	B	494	LYS	27.9
1	B	472	GLU	27.8
1	A	42	LYS	27.8
1	A	533	GLY	27.7
1	A	649	PRO	27.7
2	H	210	THR	27.7
1	A	595	GLN	27.7
1	B	386	ASN	27.7
1	B	371	THR	27.6
1	A	481	THR	27.5
1	A	263	GLU	27.5
1	B	61	LEU	27.5
3	C	52	THR	27.4
2	H	95	PRO	27.4
3	D	29	ALA	27.4

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Mol	Chain	Res	Type	RSRZ
1	A	154	LEU	27.4
1	A	447	LYS	27.4
2	H	237	GLU	27.3
1	B	541	MET	27.3
1	A	456	HIS	27.3
2	H	164	ALA	27.3
2	G	24	MET	27.3
1	A	763	MET	27.3
1	B	717	LEU	27.3
1	A	444	LEU	27.3
3	D	52	THR	27.2
1	B	279	PHE	27.2
1	B	502	LEU	27.2
3	C	50	THR	27.1
3	D	44	LEU	27.1
1	B	537	PHE	27.1
1	B	504	GLY	27.1
1	B	563	MET	27.1
1	B	278	LEU	27.1
1	B	531	ASP	27.0
3	C	44	LEU	27.0
1	B	262	THR	26.9
1	A	480	VAL	26.9
2	H	126	VAL	26.9
1	A	598	GLN	26.9
1	B	535	THR	26.9
1	B	272	ALA	26.8
1	A	261	LEU	26.7
1	A	626	ILE	26.7
1	B	495	LEU	26.7
4	F	62	PHE	26.6
2	H	303	MET	26.5
3	C	57	PHE	26.5
3	D	45	TRP	26.4
1	A	262	THR	26.4
3	C	45	TRP	26.3
1	B	383	ASN	26.3
1	A	627	VAL	26.3
2	G	26	VAL	26.3
2	G	35	PRO	26.2
1	B	770	GLU	26.2
2	H	319	ILE	26.2

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Mol	Chain	Res	Type	RSRZ
1	B	186	ARG	26.2
2	H	324	TYR	26.1
1	A	689	MET	26.1
1	A	199	ARG	26.0
1	B	558	LEU	26.0
3	C	59	LEU	25.9
1	A	556	ALA	25.9
2	H	172	ILE	25.9
2	H	130	GLY	25.8
2	H	370	PHE	25.8
1	A	608	GLU	25.8
1	A	486	MET	25.8
4	F	22	LEU	25.8
1	A	43	HIS	25.7
1	A	277	ASN	25.7
1	B	482	ILE	25.7
1	A	736	GLN	25.7
3	D	55	ILE	25.7
2	H	297	ILE	25.7
1	A	36	LEU	25.7
1	A	61	LEU	25.7
3	C	49	LEU	25.6
1	A	357	PHE	25.6
1	A	700	GLU	25.6
2	H	373	LEU	25.6
1	B	496	GLY	25.6
1	A	691	ARG	25.5
1	A	153	GLY	25.5
1	A	476	GLN	25.5
2	H	153	SER	25.5
3	D	37	SER	25.5
2	G	34	ILE	25.4
1	B	28	ALA	25.4
1	A	122	LYS	25.4
1	A	200	PRO	25.4
1	B	399	VAL	25.3
1	A	319	PHE	25.3
1	B	392	ILE	25.3
1	B	568	PRO	25.2
1	A	449	LEU	25.2
1	A	521	GLN	25.2
1	B	501	GLU	25.2

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Mol	Chain	Res	Type	RSRZ
1	B	456	HIS	25.2
1	B	267	THR	25.2
2	G	327	THR	25.2
3	C	58	ILE	25.1
1	B	553	ARG	25.1
1	B	33	TYR	25.1
2	G	194	VAL	25.0
2	G	31	GLY	25.0
1	B	271	LYS	24.9
1	A	459	LEU	24.9
1	B	480	VAL	24.9
2	G	310	PHE	24.8
1	B	505	LEU	24.7
1	B	407	ILE	24.7
1	A	675	ASP	24.7
1	A	505	LEU	24.7
1	A	276	ASP	24.6
1	A	213	LEU	24.6
2	H	224	LEU	24.6
4	E	26	ARG	24.6
1	A	686	GLU	24.6
1	B	465	GLU	24.6
2	H	129	LEU	24.5
2	H	154	PHE	24.5
1	B	350	MET	24.4
2	G	351	ARG	24.4
1	B	408	TYR	24.4
2	H	125	THR	24.3
1	B	63	VAL	24.3
1	A	379	GLU	24.3
1	B	758	ALA	24.2
1	B	562	GLY	24.2
2	H	220	LEU	24.2
4	F	61	LEU	24.2
2	H	311	TYR	24.1
2	H	320	VAL	24.1
4	E	63	LEU	24.1
2	G	279	GLN	24.1
2	H	152	ILE	24.1
1	A	209	VAL	24.1
2	G	197	PHE	24.0
3	D	28	LYS	24.0

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Mol	Chain	Res	Type	RSRZ
2	H	213	ILE	24.0
1	A	684	MET	24.0
1	A	484	THR	24.0
2	H	133	PHE	24.0
1	A	119	LEU	24.0
1	A	765	GLU	24.0
2	H	312	ASN	24.0
1	A	636	GLU	23.9
1	A	35	ASN	23.9
1	A	443	GLU	23.9
2	H	136	ARG	23.9
1	A	41	LEU	23.9
1	B	99	GLU	23.9
1	B	406	LEU	23.8
2	H	131	ILE	23.8
2	H	165	GLY	23.8
1	B	463	ASN	23.8
2	H	212	ASP	23.8
4	F	18	ILE	23.8
1	A	594	LYS	23.8
1	B	411	MET	23.8
1	B	29	ILE	23.8
3	C	35	ILE	23.6
2	H	38	GLY	23.6
2	H	27	ILE	23.6
1	B	397	PRO	23.6
1	B	22	ILE	23.5
2	H	159	VAL	23.5
2	G	94	ILE	23.5
2	G	321	PHE	23.5
1	B	65	ALA	23.5
1	A	485	ASN	23.4
3	C	51	PHE	23.4
1	A	637	ARG	23.4
1	A	62	LEU	23.4
1	A	59	ASP	23.3
1	A	690	ASP	23.3
4	F	21	LEU	23.3
2	H	349	GLY	23.3
2	H	91	THR	23.3
2	G	285	PRO	23.3
2	H	371	GLY	23.3

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Mol	Chain	Res	Type	RSRZ
1	A	360	TYR	23.3
1	B	285	ALA	23.2
4	E	21	LEU	23.2
4	E	27	GLY	23.2
2	G	308	ALA	23.2
2	H	40	ASN	23.2
1	B	38	ASP	23.1
2	H	132	ALA	23.1
2	G	331	ILE	23.1
1	B	459	LEU	23.1
4	E	20	THR	23.1
1	B	67	ALA	23.0
1	B	506	ALA	23.0
1	A	518	ILE	22.9
2	H	305	GLN	22.9
1	A	519	ASP	22.9
1	A	597	LEU	22.9
2	G	97	LEU	22.9
1	B	44	LYS	22.9
2	H	225	ILE	22.8
1	A	123	GLY	22.8
3	C	38	LEU	22.8
1	B	507	VAL	22.8
1	A	482	ILE	22.7
1	B	559	ASP	22.7
1	A	189	MET	22.7
1	A	446	SER	22.6
2	G	131	ILE	22.6
1	A	641	ALA	22.6
2	H	342	LYS	22.5
1	B	34	GLU	22.5
1	B	263	GLU	22.5
4	E	66	ALA	22.5
2	G	333	PRO	22.5
2	G	228	ILE	22.5
1	A	57	THR	22.5
1	A	146	GLU	22.5
1	A	761	GLU	22.4
1	A	429	GLY	22.4
2	H	226	ILE	22.4
1	B	37	SER	22.4
1	B	396	ARG	22.3

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Mol	Chain	Res	Type	RSRZ
1	B	391	THR	22.3
1	A	134	ALA	22.3
1	B	208	GLU	22.3
1	B	569	ILE	22.3
1	B	19	TYR	22.3
1	A	699	LYS	22.3
1	B	409	ARG	22.2
1	A	694	THR	22.2
2	G	221	ILE	22.2
3	D	34	ILE	22.2
2	G	219	LEU	22.2
2	H	238	ALA	22.2
2	G	195	ALA	22.1
2	H	287	THR	22.1
2	H	223	ALA	22.1
2	H	325	PHE	22.0
2	G	280	ALA	22.0
1	A	317	ASP	22.0
2	H	301	ALA	22.0
2	H	134	TRP	21.9
2	G	23	LEU	21.9
1	A	403	ARG	21.9
1	B	180	LEU	21.9
1	B	551	ALA	21.8
4	E	22	LEU	21.8
1	A	698	GLU	21.8
2	H	298	LYS	21.8
1	B	540	SER	21.8
3	C	39	ALA	21.8
1	B	508	VAL	21.7
2	H	323	THR	21.7
1	B	431	PRO	21.7
1	B	510	THR	21.7
1	A	231	THR	21.7
2	H	304	PHE	21.7
1	B	59	ASP	21.7
2	G	353	GLY	21.6
1	B	432	VAL	21.6
1	A	688	ILE	21.6
1	A	208	GLU	21.6
1	B	288	HIS	21.6
2	G	349	GLY	21.6

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Mol	Chain	Res	Type	RSRZ
3	C	34	ILE	21.5
1	B	183	ASP	21.5
1	B	720	VAL	21.5
1	B	760	PHE	21.5
1	B	429	GLY	21.5
1	A	606	GLN	21.5
1	A	126	VAL	21.5
3	D	51	PHE	21.5
1	B	223	ILE	21.5
1	B	249	ASP	21.4
1	A	747	ASN	21.4
2	H	279	GLN	21.4
1	A	633	SER	21.4
1	A	759	MET	21.4
2	G	134	TRP	21.3
1	A	511	GLU	21.3
2	H	13	GLU	21.3
3	C	56	SER	21.3
1	B	60	ASP	21.3
1	A	523	ARG	21.3
2	G	368	ILE	21.3
2	H	124	ALA	21.3
2	G	220	LEU	21.3
1	A	672	GLU	21.3
1	B	250	TYR	21.2
2	H	302	ASP	21.2
2	H	169	LEU	21.2
1	A	377	GLU	21.2
4	F	17	ILE	21.2
2	G	136	ARG	21.2
1	B	32	ASP	21.1
1	A	718	ARG	21.1
1	A	188	ASN	21.1
1	A	561	PHE	21.1
1	A	455	PRO	21.1
1	A	477	LYS	21.1
2	H	341	HIS	21.1
1	B	528	ARG	21.1
1	A	425	ARG	21.1
1	B	410	THR	21.0
2	H	343	ALA	21.0
2	G	145	PRO	21.0

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Mol	Chain	Res	Type	RSRZ
2	H	173	ALA	21.0
1	A	227	ALA	20.9
2	H	227	ALA	20.9
1	B	42	LYS	20.9
2	G	288	LEU	20.9
4	E	25	GLY	20.8
1	B	264	GLU	20.8
1	B	552	GLU	20.8
1	A	275	ILE	20.8
1	A	55	GLY	20.8
2	H	307	GLY	20.8
1	B	771	VAL	20.8
2	H	344	GLY	20.7
2	H	295	PRO	20.7
1	A	695	LYS	20.7
2	G	205	TYR	20.7
1	B	530	GLY	20.7
2	H	211	GLY	20.7
1	A	610	ILE	20.7
2	G	284	ILE	20.7
1	A	40	ALA	20.6
1	A	175	SER	20.6
1	B	428	THR	20.6
2	G	307	GLY	20.5
1	A	693	ILE	20.5
1	A	432	VAL	20.5
1	B	23	ALA	20.5
1	A	133	LEU	20.5
2	G	90	LEU	20.5
1	B	477	LYS	20.5
2	H	368	ILE	20.5
2	H	135	ILE	20.4
1	B	64	GLU	20.4
1	B	405	ASP	20.4
1	B	576	ARG	20.4
1	B	372	GLY	20.4
1	A	252	TYR	20.4
1	B	716	VAL	20.4
2	H	222	ILE	20.4
2	G	227	ALA	20.4
1	B	356	THR	20.4
3	D	48	ASP	20.3

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Mol	Chain	Res	Type	RSRZ
1	B	772	ALA	20.3
1	B	25	ASP	20.3
2	H	94	ILE	20.3
2	G	37	PRO	20.3
1	A	361	PHE	20.3
1	A	516	ARG	20.2
2	H	306	PRO	20.2
2	H	15	ARG	20.2
1	B	653	LYS	20.2
1	B	652	TRP	20.2
2	H	209	LYS	20.2
2	G	229	ILE	20.1
1	A	333	LEU	20.0
2	G	343	ALA	20.0
2	G	332	ASN	20.0
2	H	32	SER	19.9
1	A	696	TYR	19.9
1	B	100	MET	19.9
2	H	168	PHE	19.9
1	B	43	HIS	19.9
1	A	514	GLU	19.9
1	B	370	MET	19.9
2	H	163	VAL	19.8
1	B	284	VAL	19.8
1	B	40	ALA	19.8
1	B	373	THR	19.8
1	B	430	GLN	19.8
1	A	229	LYS	19.8
4	F	24	LYS	19.8
1	A	406	LEU	19.8
1	A	171	ASP	19.8
1	A	555	MET	19.8
1	A	148	LEU	19.7
2	H	314	LEU	19.7
1	B	458	VAL	19.7
1	A	332	GLY	19.7
1	B	45	THR	19.7
1	A	504	GLY	19.7
3	C	32	SER	19.7
2	H	326	TYR	19.7
2	G	318	PHE	19.7
1	B	387	MET	19.7

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Mol	Chain	Res	Type	RSRZ
2	G	133	PHE	19.7
1	A	678	GLY	19.7
1	A	269	ALA	19.6
2	G	218	LEU	19.6
1	A	183	ASP	19.6
3	C	41	GLY	19.6
1	A	71	GLU	19.5
2	H	321	PHE	19.5
1	A	642	TYR	19.5
1	B	275	ILE	19.5
2	G	89	LEU	19.5
1	B	188	ASN	19.4
4	F	63	LEU	19.4
2	H	137	GLY	19.4
1	A	187	ASP	19.4
2	H	149	ASN	19.4
1	B	51	ARG	19.4
2	G	91	THR	19.3
2	G	191	ALA	19.3
1	B	27	ASP	19.3
1	A	450	LYS	19.3
1	A	121	GLY	19.3
1	A	417	ALA	19.3
2	G	319	ILE	19.3
2	G	166	THR	19.2
1	A	60	ASP	19.2
1	A	378	GLU	19.2
2	G	126	VAL	19.2
1	A	428	THR	19.2
2	G	98	GLN	19.2
1	A	540	SER	19.1
1	A	370	MET	19.1
2	G	326	TYR	19.1
1	B	723	LYS	19.1
2	H	207	LYS	19.1
2	H	96	SER	19.1
2	H	161	THR	19.1
2	G	13	GLU	19.1
2	G	202	ILE	19.1
2	G	88	GLN	19.1
1	B	503	GLY	19.1
1	B	624	ARG	19.1

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Mol	Chain	Res	Type	RSRZ
3	C	48	ASP	19.1
3	C	60	SER	19.1
2	H	351	ARG	19.1
1	A	64	GLU	19.0
1	B	479	ALA	19.0
2	G	240	ARG	19.0
1	B	445	ILE	19.0
2	H	64	GLY	19.0
1	A	634	SER	19.0
4	E	18	ILE	19.0
1	B	384	ILE	19.0
1	A	475	GLY	19.0
2	H	35	PRO	18.9
4	F	16	LEU	18.9
3	C	33	VAL	18.9
1	A	673	LYS	18.9
2	G	36	ILE	18.9
1	B	560	ARG	18.9
1	B	50	GLU	18.9
1	A	458	VAL	18.8
2	H	175	ARG	18.8
4	E	67	LEU	18.8
2	G	93	ALA	18.8
2	H	208	VAL	18.8
4	F	59	GLY	18.8
2	H	205	TYR	18.7
1	B	462	LYS	18.7
2	H	100	LEU	18.7
1	A	184	TYR	18.7
1	A	251	THR	18.7
1	A	507	VAL	18.7
1	A	501	GLU	18.7
2	G	348	PRO	18.7
2	G	158	THR	18.6
1	A	460	ASN	18.6
2	H	278	ALA	18.6
1	A	419	ALA	18.6
1	B	626	ILE	18.6
2	H	266	LYS	18.6
2	G	162	LEU	18.6
2	H	128	SER	18.6
1	A	653	LYS	18.5

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Mol	Chain	Res	Type	RSRZ
2	G	25	PHE	18.5
2	G	286	SER	18.5
2	H	98	GLN	18.5
1	B	509	GLY	18.5
2	G	309	ILE	18.5
1	A	733	GLN	18.5
1	A	676	ILE	18.5
1	B	400	ARG	18.5
1	B	273	PHE	18.5
2	G	70	LEU	18.5
3	C	36	PHE	18.4
4	E	19	SER	18.4
2	H	39	ILE	18.4
1	B	36	LEU	18.4
1	A	692	ILE	18.4
1	A	434	VAL	18.4
1	A	720	VAL	18.3
1	A	331	GLU	18.3
2	G	148	GLU	18.3
1	A	685	LEU	18.3
1	A	387	MET	18.3
2	H	308	ALA	18.3
2	G	128	SER	18.3
1	A	424	GLN	18.3
2	G	112	ILE	18.3
3	C	40	ILE	18.2
2	H	291	PHE	18.2
1	B	525	ARG	18.2
2	G	410	THR	18.2
2	G	320	VAL	18.2
1	A	768	GLU	18.2
1	A	565	ASP	18.2
3	C	37	SER	18.1
1	B	625	GLU	18.1
1	B	732	ASP	18.1
1	B	712	GLU	18.1
1	B	189	MET	18.1
1	A	358	GLN	18.1
1	A	494	LYS	18.1
1	A	186	ARG	18.1
1	A	346	GLN	18.0
4	F	23	GLN	18.0

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Mol	Chain	Res	Type	RSRZ
1	A	442	SER	17.9
1	A	596	LEU	17.9
1	B	7	LYS	17.9
1	A	411	MET	17.9
2	G	95	PRO	17.9
1	A	532	PRO	17.8
2	G	222	ILE	17.8
1	B	47	GLU	17.8
1	B	221	LEU	17.8
1	B	381	PHE	17.8
1	A	697	ASN	17.7
1	B	498	GLY	17.7
1	A	506	ALA	17.7
3	D	47	LEU	17.7
1	B	442	SER	17.7
1	B	181	GLY	17.7
3	D	32	SER	17.7
1	A	226	GLN	17.7
1	A	198	GLN	17.6
2	G	225	ILE	17.6
1	A	412	GLU	17.6
2	H	71	THR	17.6
1	B	187	ASP	17.6
2	G	224	LEU	17.6
1	A	679	LYS	17.6
1	B	185	LEU	17.5
1	B	527	GLY	17.5
2	H	97	LEU	17.5
1	A	401	ASP	17.5
1	B	212	ILE	17.5
2	H	296	PHE	17.5
2	G	278	ALA	17.4
1	A	318	SER	17.4
1	B	48	PHE	17.4
2	H	206	GLU	17.4
2	G	302	ASP	17.4
4	E	62	PHE	17.4
2	H	418	LEU	17.4
1	A	502	LEU	17.4
1	A	386	ASN	17.4
2	H	92	VAL	17.3
1	A	721	ASP	17.3

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Mol	Chain	Res	Type	RSRZ
1	A	500	LYS	17.3
1	A	159	MET	17.3
1	A	513	HIS	17.3
2	H	292	VAL	17.3
1	A	593	ARG	17.3
1	A	152	VAL	17.2
1	A	115	TYR	17.2
1	A	433	LEU	17.2
1	A	674	SER	17.2
1	A	151	THR	17.2
1	A	211	SER	17.2
2	G	12	LYS	17.2
1	A	767	ILE	17.2
1	B	680	GLU	17.2
2	G	92	VAL	17.2
1	B	579	GLU	17.2
1	A	611	TYR	17.2
2	G	306	PRO	17.2
1	A	702	GLN	17.1
1	A	348	GLU	17.1
2	G	14	LEU	17.1
1	A	440	GLU	17.1
1	A	176	THR	17.1
1	A	704	GLY	17.1
1	A	38	ASP	17.1
1	A	418	VAL	17.1
2	G	328	ALA	17.1
1	A	651	GLU	17.1
2	H	228	ILE	17.1
1	A	422	VAL	17.1
2	G	325	PHE	17.1
1	A	764	ILE	17.0
2	H	369	PHE	17.0
1	B	35	ASN	17.0
1	A	203	PHE	17.0
1	A	400	ARG	17.0
1	A	508	VAL	17.0
1	A	56	ALA	17.0
2	G	253	ARG	17.0
1	A	270	GLU	17.0
1	B	443	GLU	16.9
1	B	357	PHE	16.9

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Mol	Chain	Res	Type	RSRZ
1	B	605	GLN	16.9
2	G	287	THR	16.9
1	B	656	GLY	16.9
1	A	758	ALA	16.8
1	B	434	VAL	16.8
2	H	56	PHE	16.8
1	A	466	ARG	16.8
1	A	613	GLN	16.8
2	H	367	LEU	16.7
1	A	185	LEU	16.7
1	B	754	MET	16.7
1	B	672	GLU	16.7
1	B	755	GLU	16.7
1	B	276	ASP	16.7
4	E	65	LEU	16.7
1	A	707	GLN	16.7
1	A	677	PHE	16.6
2	G	329	VAL	16.6
2	H	253	ARG	16.6
1	A	454	ILE	16.6
1	B	71	GLU	16.6
1	B	721	ASP	16.6
2	G	254	GLN	16.6
2	H	127	GLN	16.5
2	G	330	LEU	16.5
1	A	722	SER	16.5
2	H	162	LEU	16.5
2	H	236	GLN	16.5
2	G	32	SER	16.5
1	A	274	GLY	16.5
2	G	167	MET	16.5
2	G	71	THR	16.4
1	B	657	LEU	16.4
1	A	214	ILE	16.4
2	G	303	MET	16.4
1	A	652	TRP	16.4
2	H	181	ILE	16.4
1	B	736	GLN	16.4
2	G	289	LEU	16.4
3	C	30	THR	16.4
2	G	193	ILE	16.3
1	A	408	TYR	16.3

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Mol	Chain	Res	Type	RSRZ
1	A	407	ILE	16.3
1	A	414	LYS	16.3
1	A	423	ALA	16.3
1	A	427	MET	16.3
1	A	345	ILE	16.3
1	A	155	ASN	16.3
1	B	441	THR	16.3
4	E	56	TYR	16.2
1	B	282	LYS	16.2
1	B	49	LYS	16.2
1	A	605	GLN	16.1
2	G	226	ILE	16.1
1	A	385	TYR	16.1
1	A	416	LYS	16.1
3	C	62	ARG	16.1
1	A	65	ALA	16.1
2	H	138	GLN	16.1
1	B	666	LEU	16.1
1	A	582	GLN	16.1
2	G	163	VAL	16.1
1	A	564	ASP	16.1
1	A	179	GLU	16.1
1	B	722	SER	16.1
4	F	15	VAL	16.1
4	E	58	LEU	16.1
2	H	322	PHE	16.0
1	A	737	GLY	16.0
3	C	29	ALA	16.0
1	A	383	ASN	16.0
2	H	282	LEU	16.0
2	H	170	VAL	15.9
2	G	86	MET	15.9
1	A	356	THR	15.9
1	A	260	GLN	15.9
1	B	24	ASN	15.9
1	A	671	LEU	15.9
2	G	379	ALA	15.8
1	B	524	GLY	15.8
2	G	334	VAL	15.8
3	D	56	SER	15.8
3	C	61	LEU	15.8
1	B	483	ALA	15.8

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Mol	Chain	Res	Type	RSRZ
1	A	271	LYS	15.8
1	A	131	GLU	15.7
1	A	723	LYS	15.7
2	H	284	ILE	15.7
1	B	731	MET	15.7
1	A	683	GLU	15.7
1	B	225	GLY	15.7
1	B	444	LEU	15.7
4	E	55	THR	15.6
1	A	225	GLY	15.6
2	H	214	GLY	15.6
2	G	369	PHE	15.6
1	A	719	ALA	15.6
2	H	139	VAL	15.6
1	B	773	LYS	15.6
2	H	123	VAL	15.6
1	A	250	TYR	15.6
2	G	192	GLY	15.6
1	A	74	ARG	15.6
2	H	366	ARG	15.6
3	C	42	VAL	15.5
4	E	17	ILE	15.5
1	B	320	THR	15.5
1	A	739	HIS	15.5
1	A	640	ALA	15.5
2	H	293	GLN	15.5
2	G	230	VAL	15.5
2	G	22	LEU	15.5
2	H	14	LEU	15.5
1	A	760	PHE	15.5
2	H	148	GLU	15.4
1	A	602	VAL	15.4
1	A	230	SER	15.4
1	A	180	LEU	15.4
1	A	463	ASN	15.4
2	G	159	VAL	15.4
2	G	380	LEU	15.4
1	A	708	MET	15.4
1	A	473	GLU	15.4
1	A	202	HIS	15.4
1	A	738	ILE	15.4
1	B	401	ASP	15.3

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Mol	Chain	Res	Type	RSRZ
1	A	334	HIS	15.3
1	B	349	SER	15.3
2	H	281	LEU	15.3
1	B	344	GLU	15.3
1	A	413	GLY	15.3
1	A	201	LEU	15.3
2	H	150	PRO	15.3
2	H	283	LEU	15.3
1	A	728	ILE	15.2
2	H	286	SER	15.2
1	B	427	MET	15.2
1	A	37	SER	15.2
2	H	280	ALA	15.2
2	H	414	ILE	15.2
1	B	68	VAL	15.2
2	H	59	TYR	15.2
2	G	216	LEU	15.2
1	A	329	TYR	15.2
2	H	327	THR	15.2
1	B	454	ILE	15.2
1	B	573	MET	15.2
1	B	21	LYS	15.2
1	A	492	ASP	15.1
2	H	65	GLY	15.1
1	B	210	ASP	15.1
4	E	64	VAL	15.1
1	B	66	PHE	15.1
1	B	417	ALA	15.1
1	B	261	LEU	15.1
2	G	347	ILE	15.1
1	A	599	TYR	15.1
1	B	654	LEU	15.1
2	G	196	ASN	15.0
2	G	127	GLN	15.0
1	B	733	GLN	15.0
2	G	301	ALA	15.0
1	B	227	ALA	15.0
1	A	583	LYS	15.0
1	B	577	ALA	15.0
1	A	330	SER	15.0
2	H	37	PRO	15.0
2	G	154	PHE	15.0

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Mol	Chain	Res	Type	RSRZ
1	A	603	LEU	14.9
1	B	325	LYS	14.9
2	H	317	THR	14.9
1	B	607	ARG	14.9
1	B	248	LYS	14.9
1	B	287	ASN	14.9
1	B	222	ILE	14.9
1	A	359	ASN	14.8
1	B	39	ASP	14.8
2	G	204	PHE	14.8
1	A	515	SER	14.8
1	A	735	ARG	14.8
1	A	624	ARG	14.8
1	B	621	GLU	14.7
2	G	231	GLY	14.7
1	A	607	ARG	14.7
1	B	190	VAL	14.7
1	A	181	GLY	14.7
1	B	426	TYR	14.7
1	A	643	THR	14.7
1	A	404	PRO	14.7
4	E	60	ALA	14.7
2	H	63	SER	14.6
4	F	56	TYR	14.6
1	A	437	VAL	14.6
1	B	15	THR	14.6
1	A	488	GLY	14.6
1	B	52	LEU	14.6
1	B	351	THR	14.6
2	G	164	ALA	14.6
1	B	679	LYS	14.6
1	B	348	GLU	14.6
2	G	408	LEU	14.6
2	G	378	ILE	14.5
4	E	28	ASP	14.5
1	B	18	ARG	14.5
2	G	412	ARG	14.5
2	H	60	ASP	14.5
2	H	299	VAL	14.5
2	H	348	PRO	14.5
1	A	452	LYS	14.5
1	A	253	ASP	14.5

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Mol	Chain	Res	Type	RSRZ
1	A	499	VAL	14.5
1	B	20	GLU	14.5
2	G	38	GLY	14.4
1	B	390	VAL	14.4
1	B	420	GLU	14.4
1	B	665	TYR	14.4
1	B	550	GLY	14.4
1	B	595	GLN	14.4
2	G	111	LYS	14.4
1	A	503	GLY	14.4
1	A	204	ALA	14.4
1	B	228	ALA	14.4
4	E	57	TRP	14.4
1	A	705	LYS	14.4
2	G	155	ILE	14.3
1	A	467	GLU	14.3
1	B	115	TYR	14.3
2	G	11	LEU	14.3
2	H	252	GLY	14.3
1	B	455	PRO	14.3
1	B	412	GLU	14.3
2	H	12	LYS	14.3
1	A	362	ARG	14.2
1	B	12	THR	14.2
1	B	53	GLU	14.2
2	G	255	LEU	14.2
2	G	201	VAL	14.2
1	A	462	LYS	14.2
1	A	524	GLY	14.2
2	G	161	THR	14.2
2	G	376	SER	14.2
3	C	31	ILE	14.2
2	H	177	THR	14.2
1	A	655	ASP	14.2
1	A	63	VAL	14.2
1	A	766	SER	14.2
1	B	734	LEU	14.2
1	B	561	PHE	14.1
2	G	234	TYR	14.1
1	B	724	TRP	14.1
2	H	26	VAL	14.1
1	A	495	LEU	14.1

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Mol	Chain	Res	Type	RSRZ
1	A	601	ASP	14.1
1	B	54	LYS	14.1
1	A	39	ASP	14.1
2	H	239	GLU	14.1
2	G	144	ILE	14.1
1	A	344	GLU	14.1
1	B	673	LYS	14.1
1	B	58	THR	14.1
1	B	487	ALA	14.1
2	G	15	ARG	14.1
1	A	421	ASP	14.0
1	A	137	ASP	14.0
1	B	211	SER	14.0
1	B	651	GLU	14.0
1	A	34	GLU	14.0
1	B	379	GLU	14.0
2	G	65	GLY	14.0
1	A	543	ASP	14.0
4	F	58	LEU	14.0
1	B	6	ASN	14.0
1	B	355	ILE	14.0
2	G	345	ALA	14.0
2	H	144	ILE	14.0
1	B	440	GLU	13.9
1	B	329	TYR	13.9
1	A	272	ALA	13.9
1	B	46	ILE	13.9
1	B	346	GLN	13.9
1	A	461	ALA	13.9
1	A	207	ASP	13.9
1	A	586	GLU	13.9
1	A	717	LEU	13.8
1	B	725	MET	13.8
1	A	147	PHE	13.8
2	G	190	PHE	13.8
1	A	471	ILE	13.8
1	A	553	ARG	13.8
2	G	232	ILE	13.8
4	E	29	VAL	13.8
1	A	703	PHE	13.8
1	A	138	ALA	13.8
2	G	129	LEU	13.8

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Mol	Chain	Res	Type	RSRZ
2	H	365	ASN	13.7
1	A	228	ALA	13.7
1	A	420	GLU	13.7
1	B	478	GLY	13.7
2	H	171	TRP	13.7
1	A	150	LEU	13.7
1	B	403	ARG	13.7
2	H	101	ALA	13.7
2	G	96	SER	13.7
1	B	714	VAL	13.7
1	B	678	GLY	13.6
1	A	178	ASN	13.6
1	A	145	PHE	13.6
1	A	33	TYR	13.6
1	A	177	ASN	13.6
1	A	234	TYR	13.6
1	A	474	ALA	13.5
1	A	612	LYS	13.5
1	A	469	GLN	13.5
4	E	52	THR	13.5
2	H	66	ASN	13.5
2	G	150	PRO	13.5
1	B	360	TYR	13.5
1	A	734	LEU	13.5
1	B	11	PRO	13.5
2	G	157	ILE	13.5
1	A	472	GLU	13.5
1	A	682	ASP	13.5
3	D	58	ILE	13.5
1	B	526	SER	13.4
1	B	511	GLU	13.4
2	G	99	ARG	13.4
2	G	377	VAL	13.4
1	A	654	LEU	13.4
1	B	247	GLU	13.4
1	A	139	GLU	13.4
2	H	67	LEU	13.4
1	A	604	ARG	13.4
1	A	206	ILE	13.4
1	B	286	LEU	13.4
2	G	261	THR	13.3
1	B	606	GLN	13.3

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Mol	Chain	Res	Type	RSRZ
4	E	16	LEU	13.3
1	B	345	ILE	13.3
2	G	149	ASN	13.3
2	H	93	ALA	13.3
1	A	468	ALA	13.3
2	G	305	GLN	13.3
2	G	147	VAL	13.3
1	A	749	LEU	13.3
1	B	543	ASP	13.2
2	G	252	GLY	13.2
2	H	195	ALA	13.2
2	H	16	GLN	13.2
1	B	753	GLN	13.2
1	B	729	ASP	13.2
1	B	776	MET	13.2
2	G	372	ALA	13.2
1	B	570	GLN	13.2
1	B	251	THR	13.2
2	H	199	ASN	13.2
1	B	14	ARG	13.2
1	B	229	LYS	13.2
1	B	671	LEU	13.2
1	A	542	GLU	13.1
1	B	102	THR	13.1
1	B	608	GLU	13.1
1	A	600	ASP	13.1
1	B	255	LYS	13.1
1	B	404	PRO	13.1
2	G	217	THR	13.1
1	A	656	GLY	13.1
2	G	87	MET	13.1
1	A	136	ARG	13.1
1	B	604	ARG	13.0
2	G	160	LEU	13.0
1	B	101	LYS	13.0
4	E	61	LEU	13.0
1	A	364	TYR	13.0
1	B	380	GLU	13.0
4	F	64	VAL	13.0
1	A	324	MET	13.0
1	B	728	ILE	13.0
1	A	135	SER	13.0

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Mol	Chain	Res	Type	RSRZ
1	A	168	TYR	13.0
2	G	409	ASP	13.0
2	G	165	GLY	12.9
1	A	149	GLY	12.9
2	H	151	GLY	12.9
1	B	627	VAL	12.9
4	F	25	GLY	12.9
1	B	425	ARG	12.9
4	E	53	LYS	12.9
2	H	316	VAL	12.9
1	B	756	GLY	12.9
1	B	727	HIS	12.8
1	B	179	GLU	12.8
2	H	267	ILE	12.8
1	A	130	ASN	12.8
1	A	584	ARG	12.8
1	A	70	ARG	12.8
1	A	487	ALA	12.7
1	B	574	VAL	12.7
1	B	277	ASN	12.7
2	H	409	ASP	12.7
3	D	57	PHE	12.7
1	A	182	PHE	12.7
1	A	114	VAL	12.7
2	H	419	ILE	12.7
2	G	156	LEU	12.6
2	H	285	PRO	12.6
1	B	178	ASN	12.6
2	G	182	GLY	12.6
2	G	146	VAL	12.6
2	H	410	THR	12.6
2	G	411	PHE	12.6
2	G	335	GLU	12.6
1	A	415	PHE	12.6
2	G	66	ASN	12.6
1	A	167	ALA	12.6
2	G	223	ALA	12.5
2	H	229	ILE	12.5
1	B	182	PHE	12.5
1	A	284	VAL	12.5
1	B	330	SER	12.5
1	A	732	ASP	12.5

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Mol	Chain	Res	Type	RSRZ
2	H	411	PHE	12.5
1	A	295	LYS	12.5
1	B	521	GLN	12.5
1	B	749	LEU	12.4
2	G	75	LEU	12.4
2	H	31	GLY	12.4
2	G	371	GLY	12.4
2	G	69	ARG	12.4
1	A	566	SER	12.4
1	A	731	MET	12.4
3	D	59	LEU	12.3
1	B	424	GLN	12.3
1	A	140	GLN	12.3
1	A	72	ALA	12.3
1	A	681	PRO	12.3
1	B	16	LEU	12.3
1	A	670	ALA	12.3
2	H	300	ILE	12.3
1	B	594	LYS	12.3
1	A	512	ARG	12.3
1	A	587	GLY	12.2
1	A	164	LYS	12.2
3	C	28	LYS	12.2
1	B	667	ASP	12.2
1	A	567	THR	12.2
2	H	196	ASN	12.2
2	H	174	ASP	12.2
1	B	176	THR	12.2
2	H	313	PHE	12.2
2	G	375	LEU	12.2
1	A	589	ASN	12.1
1	B	416	LYS	12.1
1	B	103	GLY	12.1
2	H	72	VAL	12.1
1	A	644	PRO	12.1
2	H	99	ARG	12.1
2	H	145	PRO	12.1
2	G	344	GLY	12.1
2	G	153	SER	12.0
1	B	578	VAL	12.0
2	H	90	LEU	12.0
1	A	297	HIS	12.0

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Mol	Chain	Res	Type	RSRZ
1	A	517	ARG	12.0
2	G	269	PRO	12.0
1	B	343	LEU	12.0
4	F	14	VAL	12.0
1	B	757	PHE	12.0
2	G	10	GLU	12.0
1	A	169	ALA	12.0
2	H	142	LYS	12.0
1	A	554	THR	12.0
1	A	299	ALA	12.0
2	H	87	MET	11.9
1	B	354	THR	11.9
1	B	359	ASN	11.9
1	A	233	LEU	11.9
1	A	190	VAL	11.9
1	A	748	PRO	11.9
2	H	390	ASN	11.9
2	G	233	VAL	11.9
1	A	75	ARG	11.9
2	H	198	PRO	11.8
1	A	335	GLN	11.8
1	A	525	ARG	11.8
2	H	388	TRP	11.8
1	A	724	TRP	11.8
1	B	523	ARG	11.8
1	B	98	ALA	11.8
1	B	224	SER	11.8
1	A	210	ASP	11.8
1	A	706	GLU	11.8
1	B	630	MET	11.8
1	A	590	PHE	11.7
1	A	367	LEU	11.7
1	A	141	MET	11.7
1	A	247	GLU	11.7
1	B	226	GLN	11.7
1	A	757	PHE	11.7
2	G	19	ILE	11.7
1	A	531	ASP	11.7
1	B	116	LEU	11.6
2	H	310	PHE	11.6
2	G	336	LEU	11.6
1	B	675	ASP	11.6

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Mol	Chain	Res	Type	RSRZ
2	H	318	PHE	11.6
2	H	36	ILE	11.6
1	B	664	THR	11.6
1	B	611	TYR	11.6
2	G	67	LEU	11.6
1	B	334	HIS	11.6
2	H	76	GLY	11.6
2	H	57	ALA	11.5
1	A	197	VAL	11.5
1	B	622	ASN	11.5
1	B	378	GLU	11.5
2	G	110	TYR	11.5
1	A	371	THR	11.5
1	A	465	GLU	11.5
1	A	725	MET	11.5
1	A	127	VAL	11.5
1	B	660	LEU	11.5
2	G	239	GLU	11.5
4	E	54	ALA	11.5
1	A	366	LYS	11.5
1	B	8	MET	11.5
1	B	708	MET	11.5
1	B	486	MET	11.4
1	B	461	ALA	11.4
1	A	363	MET	11.4
1	A	285	ALA	11.4
1	A	160	SER	11.4
1	A	680	GLU	11.4
1	B	493	ILE	11.4
1	A	755	GLU	11.4
1	A	132	TYR	11.3
1	B	414	LYS	11.3
2	H	374	PHE	11.3
1	A	304	VAL	11.3
4	E	37	MET	11.3
1	B	448	LEU	11.3
1	A	349	SER	11.3
1	A	111	THR	11.3
2	G	414	ILE	11.3
2	H	375	LEU	11.3
1	A	470	ILE	11.3
1	A	224	SER	11.3

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Mol	Chain	Res	Type	RSRZ
1	A	296	ALA	11.3
1	B	492	ASP	11.3
1	A	68	VAL	11.3
1	B	778	ALA	11.3
1	A	246	ALA	11.3
1	B	774	PHE	11.2
2	H	309	ILE	11.2
1	A	464	HIS	11.2
2	G	428	ARG	11.2
2	G	209	LYS	11.2
2	G	298	LYS	11.2
1	B	529	GLN	11.2
1	A	438	ALA	11.2
1	B	319	PHE	11.2
1	A	727	HIS	11.1
1	B	777	LYS	11.1
4	E	59	GLY	11.1
4	F	48	GLU	11.1
2	H	62	PHE	11.1
1	A	355	ILE	11.1
1	A	323	LEU	11.1
2	G	370	PHE	11.1
1	A	255	LYS	11.1
1	B	143	LYS	11.1
2	G	64	GLY	11.1
1	B	177	ASN	11.1
1	B	709	ARG	11.0
1	B	668	GLU	11.0
1	A	316	VAL	11.0
1	B	677	PHE	11.0
1	B	87	MET	11.0
2	H	25	PHE	11.0
1	B	484	THR	11.0
1	A	541	MET	11.0
2	H	179	LYS	11.0
1	B	735	ARG	11.0
1	A	751	GLU	10.9
1	B	676	ILE	10.9
1	B	413	GLY	10.9
1	B	674	SER	10.9
2	G	130	GLY	10.9
2	H	180	GLY	10.9

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Mol	Chain	Res	Type	RSRZ
1	A	410	THR	10.9
1	B	93	HIS	10.9
1	A	21	LYS	10.9
2	H	11	LEU	10.8
1	B	609	VAL	10.8
1	B	358	GLN	10.8
2	H	251	VAL	10.8
2	G	16	GLN	10.8
1	B	421	ASP	10.8
1	A	321	GLY	10.8
1	B	13	LYS	10.8
1	B	55	GLY	10.8
1	A	496	GLY	10.8
4	E	69	LEU	10.8
4	F	39	GLN	10.7
1	B	377	GLU	10.7
1	A	205	VAL	10.7
1	B	631	ILE	10.7
2	G	238	ALA	10.7
2	G	415	GLU	10.7
2	H	70	LEU	10.7
1	A	142	GLY	10.7
1	B	730	ALA	10.7
1	B	752	TYR	10.6
1	B	289	HIS	10.6
1	B	436	THR	10.6
1	B	331	GLU	10.6
2	G	206	GLU	10.6
1	A	572	LYS	10.6
1	A	657	LEU	10.6
1	B	746	THR	10.6
1	A	451	ASN	10.6
1	B	198	GLN	10.6
2	H	234	TYR	10.6
1	B	17	ASN	10.6
1	B	214	ILE	10.5
1	B	72	ALA	10.5
1	B	395	ASN	10.5
2	H	340	LEU	10.5
2	G	79	PRO	10.5
2	H	58	LEU	10.5
4	F	67	LEU	10.5

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Mol	Chain	Res	Type	RSRZ
1	B	655	ASP	10.5
1	A	552	GLU	10.5
1	A	754	MET	10.5
1	A	347	ASN	10.5
1	A	716	VAL	10.5
1	B	324	MET	10.5
1	A	257	LYS	10.5
2	G	262	TYR	10.4
1	B	612	LYS	10.4
1	B	610	ILE	10.4
2	G	346	PHE	10.4
1	A	489	ARG	10.4
1	B	598	GLN	10.4
2	H	364	ILE	10.4
1	A	776	MET	10.4
1	A	143	LYS	10.4
2	H	389	PHE	10.4
1	A	409	ARG	10.4
1	B	333	LEU	10.4
2	G	189	ILE	10.4
1	A	726	ASP	10.3
1	B	136	ARG	10.3
2	H	417	TYR	10.3
4	F	65	LEU	10.3
1	B	711	PHE	10.3
1	B	219	THR	10.3
4	E	41	ILE	10.3
1	A	156	LEU	10.3
2	G	169	LEU	10.3
1	A	365	GLU	10.3
2	G	39	ILE	10.3
2	G	407	ALA	10.3
2	H	415	GLU	10.3
2	G	73	PHE	10.3
2	H	184	GLY	10.3
2	H	248	GLY	10.3
2	H	88	GLN	10.3
2	G	68	GLY	10.3
3	D	62	ARG	10.3
1	B	398	VAL	10.2
2	H	254	GLN	10.2
1	B	460	ASN	10.2

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Mol	Chain	Res	Type	RSRZ
1	A	581	SER	10.2
1	B	90	VAL	10.2
1	B	352	LEU	10.2
1	B	669	GLY	10.2
1	A	196	MET	10.2
4	E	48	GLU	10.2
1	A	69	VAL	10.2
1	A	372	GLY	10.2
2	G	235	VAL	10.2
1	B	438	ALA	10.1
1	B	601	ASP	10.1
1	B	423	ALA	10.1
1	A	715	ILE	10.1
2	H	143	GLY	10.1
2	H	193	ILE	10.1
1	A	161	LYS	10.1
1	B	575	SER	10.1
1	A	32	ASP	10.1
2	H	413	GLN	10.1
2	G	21	THR	10.0
2	G	152	ILE	10.0
2	G	296	PHE	10.0
1	A	67	ALA	10.0
4	F	37	MET	10.0
1	A	248	LYS	10.0
1	B	603	LEU	10.0
1	A	585	VAL	10.0
1	B	661	ILE	10.0
2	H	178	GLU	10.0
1	B	393	PRO	9.9
1	A	144	ILE	9.9
1	A	170	ALA	9.9
2	H	197	PHE	9.9
2	H	182	GLY	9.9
1	B	113	PRO	9.9
1	B	419	ALA	9.9
4	F	66	ALA	9.9
1	A	298	VAL	9.9
1	A	129	VAL	9.9
1	B	726	ASP	9.9
2	G	413	GLN	9.9
1	A	258	ALA	9.9

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Mol	Chain	Res	Type	RSRZ
2	G	74	ALA	9.9
1	B	335	GLN	9.8
1	B	449	LEU	9.8
1	A	107	THR	9.8
4	F	49	THR	9.8
4	E	40	SER	9.8
1	B	616	GLU	9.8
1	B	744	ALA	9.8
1	B	580	SER	9.8
3	D	61	LEU	9.8
1	B	737	GLY	9.8
1	B	713	LYS	9.8
2	G	188	ILE	9.8
4	F	46	GLY	9.8
1	B	146	GLU	9.8
4	F	50	ILE	9.8
2	G	76	GLY	9.7
3	D	60	SER	9.7
2	G	210	THR	9.7
2	G	265	ILE	9.7
1	A	259	VAL	9.7
4	E	13	ALA	9.7
1	A	249	ASP	9.7
2	G	373	LEU	9.7
2	H	269	PRO	9.7
1	B	376	THR	9.7
2	H	420	GLN	9.7
1	B	600	ASP	9.6
4	E	46	GLY	9.6
2	G	242	ILE	9.6
2	H	69	ARG	9.6
1	B	546	MET	9.6
1	B	147	PHE	9.6
1	B	613	GLN	9.6
2	G	381	ILE	9.5
2	H	391	ILE	9.5
2	H	230	VAL	9.5
1	A	730	ALA	9.5
1	B	341	GLU	9.5
1	B	309	GLU	9.5
1	A	573	MET	9.5
1	A	729	ASP	9.5

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Mol	Chain	Res	Type	RSRZ
1	B	597	LEU	9.5
2	H	77	VAL	9.5
1	A	291	ASN	9.5
2	H	121	LEU	9.5
2	H	78	MET	9.5
1	B	310	ASP	9.4
1	B	84	VAL	9.4
2	G	264	PRO	9.4
1	B	230	SER	9.4
1	B	70	ARG	9.4
2	G	290	ASN	9.4
1	A	350	MET	9.4
2	H	416	THR	9.4
1	A	769	ASP	9.4
1	B	418	VAL	9.4
1	A	162	ASP	9.3
1	A	375	LYS	9.3
1	B	588	ASN	9.3
1	B	663	THR	9.3
2	G	337	ALA	9.3
1	B	706	GLU	9.3
4	E	30	GLY	9.3
1	A	22	ILE	9.3
1	B	338	GLU	9.3
2	G	405	GLY	9.3
2	H	265	ILE	9.3
2	H	412	ARG	9.3
1	B	549	PHE	9.3
1	A	288	HIS	9.2
2	H	75	LEU	9.2
1	B	94	ASP	9.2
2	G	416	THR	9.2
1	B	614	ARG	9.2
2	G	295	PRO	9.2
2	G	138	GLN	9.1
1	B	215	ASP	9.1
1	A	772	ALA	9.1
1	B	581	SER	9.1
1	A	113	PRO	9.1
1	A	756	GLY	9.1
2	H	10	GLU	9.1
1	A	369	GLY	9.1

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Mol	Chain	Res	Type	RSRZ
1	A	192	TYR	9.1
1	B	140	GLN	9.1
1	B	332	GLY	9.1
2	H	120	THR	9.1
1	A	343	LEU	9.1
1	A	568	PRO	9.1
1	B	516	ARG	9.1
1	B	347	ASN	9.1
1	B	572	LYS	9.1
1	B	117	ASN	9.1
4	E	31	ALA	9.0
1	A	750	ARG	9.0
1	B	388	GLN	9.0
2	G	170	VAL	9.0
1	A	301	GLN	9.0
1	A	405	ASP	9.0
1	B	95	GLY	9.0
1	A	294	LEU	9.0
1	A	660	LEU	9.0
2	H	242	ILE	9.0
1	B	291	ASN	9.0
2	H	231	GLY	9.0
1	A	236	GLN	9.0
1	A	623	LEU	9.0
1	B	599	TYR	9.0
2	H	345	ALA	9.0
1	B	56	ALA	9.0
1	B	522	LEU	8.9
1	A	112	LEU	8.9
1	B	69	VAL	8.9
1	B	745	GLN	8.9
4	F	57	TRP	8.9
2	G	340	LEU	8.9
4	E	39	GLN	8.9
1	B	422	VAL	8.9
1	A	439	VAL	8.9
1	B	739	HIS	8.9
1	B	10	ASP	8.9
2	H	122	PHE	8.9
1	B	520	ASN	8.9
1	B	362	ARG	8.8
1	B	213	LEU	8.8

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Mol	Chain	Res	Type	RSRZ
4	E	15	VAL	8.8
1	A	66	PHE	8.8
1	B	615	PHE	8.8
1	B	738	ILE	8.8
2	G	406	VAL	8.8
2	H	232	ILE	8.8
1	B	670	ALA	8.8
1	B	353	ALA	8.8
1	B	447	LYS	8.8
1	B	705	LYS	8.8
1	A	163	GLU	8.8
4	F	38	GLY	8.8
1	B	141	MET	8.8
2	H	376	SER	8.7
2	H	191	ALA	8.7
2	G	263	LEU	8.7
1	A	300	MET	8.7
1	B	139	GLU	8.7
1	B	394	THR	8.7
2	G	171	TRP	8.7
1	A	709	ARG	8.7
1	B	246	ALA	8.7
2	G	299	VAL	8.7
1	B	220	PRO	8.7
1	B	119	LEU	8.7
4	E	33	PHE	8.7
2	G	293	GLN	8.7
2	H	61	ILE	8.7
2	G	139	VAL	8.7
1	B	489	ARG	8.7
1	B	517	ARG	8.7
2	G	175	ARG	8.7
1	B	83	LYS	8.7
1	B	591	ASP	8.6
1	B	363	MET	8.6
1	A	292	GLN	8.6
1	A	273	PHE	8.6
1	B	375	LYS	8.6
4	F	55	THR	8.6
2	G	250	GLN	8.6
4	E	32	ALA	8.6
2	H	233	VAL	8.6

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Mol	Chain	Res	Type	RSRZ
1	A	81	PRO	8.6
1	B	593	ARG	8.6
1	A	384	ILE	8.6
2	H	74	ALA	8.6
2	H	204	PHE	8.6
4	F	44	VAL	8.6
2	H	89	LEU	8.5
1	B	446	SER	8.5
1	A	453	GLY	8.5
1	A	614	ARG	8.5
2	H	250	GLN	8.5
2	G	215	PRO	8.5
1	B	91	ALA	8.5
1	A	328	ARG	8.5
1	A	753	GLN	8.5
1	B	518	ILE	8.5
1	B	57	THR	8.5
2	G	100	LEU	8.5
1	B	750	ARG	8.4
2	G	176	ILE	8.4
1	A	588	ASN	8.4
2	H	200	ALA	8.4
2	G	211	GLY	8.4
2	G	249	ARG	8.4
4	E	70	SER	8.4
2	H	277	PHE	8.4
1	B	112	LEU	8.4
2	H	185	ALA	8.4
2	H	352	PRO	8.4
2	H	147	VAL	8.4
1	B	138	ALA	8.3
2	H	235	VAL	8.3
1	B	297	HIS	8.3
1	A	18	ARG	8.3
2	G	8	LEU	8.3
2	H	68	GLY	8.3
1	A	326	GLY	8.3
1	B	635	LEU	8.3
4	E	38	GLY	8.3
1	B	142	GLY	8.3
1	B	114	VAL	8.3
1	A	327	ARG	8.3

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Mol	Chain	Res	Type	RSRZ
2	H	249	ARG	8.3
1	B	488	GLY	8.3
2	G	374	PHE	8.3
2	H	347	ILE	8.3
1	A	752	TYR	8.3
1	B	548	ARG	8.2
2	H	328	ALA	8.2
2	G	251	VAL	8.2
1	B	105	GLY	8.2
2	H	272	VAL	8.2
2	G	247	PRO	8.2
1	B	437	VAL	8.2
1	A	128	THR	8.2
1	B	374	ALA	8.2
1	B	191	LEU	8.2
2	G	179	LYS	8.2
1	B	292	GLN	8.2
1	A	256	THR	8.2
2	G	277	PHE	8.2
1	B	342	GLY	8.1
1	B	682	ASP	8.1
2	G	40	ASN	8.1
4	F	52	THR	8.1
2	H	408	LEU	8.1
1	B	192	TYR	8.1
1	A	322	ARG	8.1
1	A	338	GLU	8.1
1	A	579	GLU	8.1
2	G	245	GLN	8.1
1	B	97	ILE	8.1
2	H	24	MET	8.1
1	A	245	LYS	8.1
1	B	485	ASN	8.1
2	G	300	ILE	8.1
2	H	79	PRO	8.1
2	G	17	LYS	8.1
2	H	363	ILE	8.1
1	A	580	SER	8.0
1	A	73	SER	8.0
1	B	702	GLN	8.0
1	A	25	ASP	8.0
4	F	26	ARG	8.0

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Mol	Chain	Res	Type	RSRZ
1	A	216	GLU	8.0
2	G	304	PHE	8.0
1	B	450	LYS	8.0
2	G	137	GLY	8.0
2	G	151	GLY	8.0
1	B	596	LEU	7.9
2	G	177	THR	7.9
2	G	248	GLY	7.9
1	B	491	THR	7.9
1	A	165	ARG	7.9
2	H	256	TYR	7.9
2	G	56	PHE	7.9
2	G	404	VAL	7.9
2	H	294	ASN	7.9
1	A	215	ASP	7.9
1	A	368	ALA	7.9
2	G	85	ILE	7.9
1	B	544	GLU	7.9
2	G	9	PHE	7.9
1	A	526	SER	7.9
2	H	194	VAL	7.8
2	G	256	TYR	7.8
2	H	264	PRO	7.8
1	B	86	LEU	7.8
2	H	378	ILE	7.8
2	G	83	ALA	7.8
2	H	240	ARG	7.8
1	A	493	ILE	7.8
1	A	376	THR	7.8
1	A	569	ILE	7.8
1	B	584	ARG	7.8
4	F	45	GLY	7.8
1	B	547	ARG	7.8
1	B	681	PRO	7.8
1	B	710	GLU	7.7
1	A	388	GLN	7.7
1	B	326	GLY	7.7
1	A	315	ILE	7.7
2	H	271	GLY	7.7
1	B	389	VAL	7.7
1	B	243	THR	7.7
1	B	402	ASP	7.7

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Mol	Chain	Res	Type	RSRZ
1	A	770	GLU	7.7
1	B	252	TYR	7.6
2	H	275	ILE	7.6
1	A	223	ILE	7.6
1	A	373	THR	7.6
1	B	590	PHE	7.6
1	B	439	VAL	7.6
2	G	183	ASN	7.6
2	G	384	LEU	7.6
2	G	77	VAL	7.6
1	A	100	MET	7.6
1	B	618	ILE	7.6
1	B	628	GLU	7.6
1	A	498	GLY	7.6
1	B	775	VAL	7.6
4	F	53	LYS	7.6
1	A	108	LEU	7.6
2	H	268	ASN	7.5
1	B	120	THR	7.5
2	G	143	GLY	7.5
1	B	104	GLU	7.5
2	H	115	TYR	7.5
1	B	586	GLU	7.5
2	G	207	LYS	7.5
1	A	648	LEU	7.5
1	B	490	GLY	7.5
1	B	361	PHE	7.5
2	G	236	GLN	7.5
2	G	382	PRO	7.5
1	A	647	GLU	7.5
2	G	101	ALA	7.5
2	G	173	ALA	7.5
2	H	73	PHE	7.5
1	B	217	ALA	7.5
2	H	192	GLY	7.5
1	A	254	ILE	7.4
1	A	99	GLU	7.4
1	A	191	LEU	7.4
1	A	592	SER	7.4
2	G	186	SER	7.4
2	G	18	PHE	7.4
1	A	20	GLU	7.4

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Mol	Chain	Res	Type	RSRZ
1	B	299	ALA	7.4
2	G	20	PHE	7.4
2	G	383	ILE	7.4
1	B	707	GLN	7.4
4	F	33	PHE	7.4
1	A	77	THR	7.4
1	A	336	ALA	7.4
2	G	168	PHE	7.4
1	A	235	VAL	7.4
1	A	490	GLY	7.4
1	A	712	GLU	7.4
2	G	291	PHE	7.4
4	F	51	LEU	7.4
2	H	17	LYS	7.3
1	B	88	GLY	7.3
1	B	137	ASP	7.3
1	B	619	ASP	7.3
2	G	174	ASP	7.3
2	G	178	GLU	7.3
2	G	61	ILE	7.3
2	H	362	ARG	7.3
2	H	81	ILE	7.3
1	B	435	GLY	7.3
2	G	185	ALA	7.3
1	A	195	GLN	7.3
2	G	187	LEU	7.3
4	F	13	ALA	7.3
1	B	92	LEU	7.2
2	G	80	TYR	7.2
1	B	629	ASN	7.2
2	H	116	THR	7.2
1	B	328	ARG	7.2
2	G	172	ILE	7.2
1	A	217	ALA	7.2
1	B	135	SER	7.2
2	H	377	VAL	7.2
1	B	415	PHE	7.2
1	B	650	GLU	7.2
2	G	109	ARG	7.2
4	E	14	VAL	7.2
1	B	89	GLY	7.2
4	E	43	GLY	7.2

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Mol	Chain	Res	Type	RSRZ
1	B	231	THR	7.2
1	B	602	VAL	7.1
1	B	632	LYS	7.1
1	B	218	ARG	7.1
1	A	577	ALA	7.1
1	B	158	SER	7.1
1	B	81	PRO	7.1
2	G	78	MET	7.1
1	A	491	THR	7.1
2	G	243	PRO	7.1
2	H	407	ALA	7.1
1	B	85	GLN	7.1
2	H	183	ASN	7.1
1	A	306	TYR	7.1
1	B	701	GLU	7.0
1	A	777	LYS	7.0
2	G	268	ASN	7.0
1	B	197	VAL	7.0
2	G	208	VAL	7.0
1	B	751	GLU	7.0
1	A	87	MET	7.0
1	A	303	ASP	7.0
2	G	259	ARG	7.0
2	G	292	VAL	7.0
2	H	119	LEU	7.0
1	A	302	LYS	7.0
1	A	220	PRO	7.0
1	B	9	PHE	7.0
1	B	216	GLU	7.0
2	H	387	VAL	6.9
4	E	44	VAL	6.9
1	B	658	VAL	6.9
1	A	98	ALA	6.9
2	G	401	LEU	6.9
1	A	497	GLU	6.9
2	H	276	ILE	6.9
1	B	133	LEU	6.9
1	B	748	PRO	6.8
1	B	321	GLY	6.8
1	B	290	ILE	6.8
2	H	80	TYR	6.8
1	B	75	ARG	6.8

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Mol	Chain	Res	Type	RSRZ
1	B	144	ILE	6.8
4	F	41	ILE	6.8
1	A	773	LYS	6.8
1	A	305	ASP	6.8
4	E	68	LEU	6.8
1	A	591	ASP	6.8
1	B	111	THR	6.8
2	G	181	ILE	6.8
2	H	270	ALA	6.8
4	E	45	GLY	6.8
1	A	83	LYS	6.8
1	B	106	LYS	6.8
1	B	311	GLY	6.7
1	B	683	GLU	6.7
2	G	266	LYS	6.7
2	H	146	VAL	6.7
1	B	339	ALA	6.7
1	A	109	THR	6.7
1	B	636	GLU	6.7
2	H	203	GLN	6.7
1	B	589	ASN	6.7
1	B	159	MET	6.7
2	G	338	GLU	6.7
2	G	417	TYR	6.7
1	B	199	ARG	6.7
2	G	385	ILE	6.6
1	B	743	TYR	6.6
2	H	189	ILE	6.6
1	A	79	MET	6.6
1	A	713	LYS	6.6
2	G	237	GLU	6.6
1	A	550	GLY	6.6
1	A	337	ILE	6.6
2	G	294	ASN	6.6
1	B	295	LYS	6.6
1	B	582	GLN	6.6
2	H	405	GLY	6.6
1	A	325	LYS	6.6
1	B	634	SER	6.6
1	A	19	TYR	6.6
2	H	392	PRO	6.6
1	A	771	VAL	6.6

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Mol	Chain	Res	Type	RSRZ
1	B	583	LYS	6.6
1	B	164	LYS	6.5
2	H	118	TYR	6.5
1	B	234	TYR	6.5
1	B	312	GLN	6.5
2	G	270	ALA	6.5
2	H	379	ALA	6.5
2	H	8	LEU	6.5
1	A	110	SER	6.5
2	H	273	ILE	6.5
1	A	399	VAL	6.5
1	B	74	ARG	6.4
1	B	519	ASP	6.4
1	A	645	ARG	6.4
1	B	740	LEU	6.4
2	G	297	ILE	6.4
1	A	289	HIS	6.4
2	H	190	PHE	6.4
1	A	166	GLU	6.3
1	A	243	THR	6.3
1	B	298	VAL	6.3
1	B	132	TYR	6.3
1	A	744	ALA	6.3
1	B	571	SER	6.3
1	A	778	ALA	6.3
1	A	287	ASN	6.3
4	F	27	GLY	6.3
1	B	96	ASN	6.3
1	A	669	GLY	6.3
1	B	453	GLY	6.3
1	B	148	LEU	6.3
2	H	140	SER	6.2
2	H	257	ALA	6.2
1	B	747	ASN	6.2
1	A	76	VAL	6.2
1	B	620	SER	6.2
2	H	406	VAL	6.2
4	E	12	ILE	6.2
4	F	36	GLY	6.2
2	H	141	PRO	6.2
2	G	72	VAL	6.2
1	B	207	ASP	6.2

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Mol	Chain	Res	Type	RSRZ
2	H	186	SER	6.1
1	B	514	GLU	6.1
1	B	82	PHE	6.1
2	G	81	ILE	6.1
1	A	158	SER	6.1
1	B	294	LEU	6.1
1	B	691	ARG	6.1
2	H	188	ILE	6.1
1	B	239	ALA	6.1
1	B	369	GLY	6.1
1	B	107	THR	6.1
1	B	202	HIS	6.1
1	A	551	ALA	6.1
1	A	17	ASN	6.0
1	B	118	ALA	6.0
1	B	232	LYS	6.0
4	F	11	ILE	6.0
2	H	241	ARG	6.0
1	B	742	ALA	5.9
1	A	157	ASN	5.9
1	B	695	LYS	5.9
1	B	201	LEU	5.9
4	E	47	VAL	5.9
2	G	400	ALA	5.9
1	A	286	LEU	5.9
1	A	26	ILE	5.9
1	B	196	MET	5.9
1	A	527	GLY	5.9
1	B	698	GLU	5.9
1	A	775	VAL	5.8
1	A	353	ALA	5.8
2	G	272	VAL	5.8
2	G	84	SER	5.8
1	A	97	ILE	5.8
1	B	694	THR	5.8
1	B	704	GLY	5.8
2	G	180	GLY	5.8
4	E	42	PHE	5.8
2	G	399	THR	5.8
4	E	11	ILE	5.8
2	G	402	ILE	5.8
1	B	587	GLY	5.8

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Mol	Chain	Res	Type	RSRZ
1	B	633	SER	5.8
2	G	339	ASN	5.8
2	H	259	ARG	5.7
4	E	51	LEU	5.7
1	A	741	ARG	5.7
1	B	545	LEU	5.7
1	B	157	ASN	5.7
1	B	238	ASN	5.7
2	G	107	TYR	5.7
2	G	184	GLY	5.7
1	B	244	LEU	5.7
2	G	212	ASP	5.7
1	A	714	VAL	5.7
1	B	336	ALA	5.7
1	B	662	ASN	5.6
1	A	354	THR	5.6
2	G	267	ILE	5.6
2	G	403	VAL	5.6
1	B	318	SER	5.6
1	B	452	LYS	5.6
2	H	117	LYS	5.6
2	H	255	LEU	5.6
1	B	585	VAL	5.6
1	A	570	GLN	5.6
1	A	293	ALA	5.6
2	H	112	ILE	5.6
1	A	23	ALA	5.6
1	B	125	HIS	5.6
1	B	110	SER	5.5
4	F	31	ALA	5.5
2	G	276	ILE	5.5
1	B	696	TYR	5.5
2	H	246	TYR	5.5
1	A	711	PHE	5.5
1	A	374	ALA	5.5
2	H	398	THR	5.5
2	G	57	ALA	5.5
4	E	8	LEU	5.5
1	B	145	PHE	5.5
2	H	9	PHE	5.5
1	A	341	GLU	5.5
1	A	571	SER	5.5

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Mol	Chain	Res	Type	RSRZ
1	A	222	ILE	5.4
2	G	246	TYR	5.4
1	B	592	SER	5.4
2	G	419	ILE	5.4
2	G	423	TYR	5.4
2	G	271	GLY	5.4
1	A	86	LEU	5.4
1	B	659	ASP	5.4
1	B	451	ASN	5.4
1	A	29	ILE	5.4
2	G	102	LYS	5.4
2	H	258	GLY	5.4
2	H	187	LEU	5.4
1	A	193	LYS	5.3
1	B	134	ALA	5.3
1	A	30	ARG	5.3
1	A	106	LYS	5.3
2	H	113	ASN	5.3
2	H	86	MET	5.3
1	A	545	LEU	5.3
2	H	262	TYR	5.3
2	G	398	THR	5.3
1	B	174	TYR	5.3
1	A	528	ARG	5.3
1	B	200	PRO	5.2
4	E	50	ILE	5.2
1	B	77	THR	5.2
4	F	32	ALA	5.2
1	B	131	GLU	5.2
2	G	82	SER	5.2
4	F	28	ASP	5.2
1	A	351	THR	5.2
2	G	106	ASP	5.2
1	A	290	ILE	5.2
4	E	34	GLY	5.2
1	A	740	LEU	5.1
1	A	85	GLN	5.1
1	B	245	LYS	5.1
1	B	327	ARG	5.1
4	E	35	GLY	5.1
2	H	202	ILE	5.1
1	A	312	GLN	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	31	GLY	5.1
1	B	690	ASP	5.1
1	A	544	GLU	5.1
2	G	63	SER	5.1
1	A	745	GLN	5.1
1	B	293	ALA	5.1
4	F	35	GLY	5.1
1	B	109	THR	5.1
1	B	233	LEU	5.1
1	A	78	GLY	5.1
2	G	244	ILE	5.1
1	A	710	GLU	5.1
1	A	218	ARG	5.1
1	B	300	MET	5.0
1	A	28	ALA	5.0
2	G	104	GLU	5.0
2	H	83	ALA	5.0
2	G	273	ILE	5.0
4	F	47	VAL	5.0
1	B	296	ALA	5.0
1	A	27	ASP	5.0
1	A	194	GLU	5.0
2	H	261	THR	5.0
1	B	367	LEU	5.0
2	H	114	GLU	5.0
4	E	49	THR	5.0
2	G	418	LEU	5.0
1	B	163	GLU	5.0
1	B	193	LYS	5.0
1	B	242	ARG	4.9
2	G	103	GLU	4.9
2	H	21	THR	4.9
1	A	244	LEU	4.9
2	G	420	GLN	4.9
2	G	260	LYS	4.9
1	B	686	GLU	4.9
1	A	529	GLN	4.9
2	G	427	VAL	4.9
4	E	36	GLY	4.9
1	B	129	VAL	4.9
1	A	95	GLY	4.9
1	B	156	LEU	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	310	ASP	4.8
1	A	578	VAL	4.8
1	B	687	LEU	4.8
4	E	9	PHE	4.8
1	A	24	ASN	4.8
1	B	236	GLN	4.8
1	B	76	VAL	4.8
2	H	82	SER	4.8
2	H	401	LEU	4.8
1	A	311	GLY	4.8
1	B	165	ARG	4.8
1	B	340	LYS	4.8
1	A	16	LEU	4.8
2	G	58	LEU	4.8
1	B	337	ILE	4.8
1	A	93	HIS	4.8
1	A	309	GLU	4.8
1	B	617	VAL	4.8
1	B	254	ILE	4.7
1	B	73	SER	4.7
1	B	323	LEU	4.7
1	B	121	GLY	4.7
1	A	661	ILE	4.7
4	E	71	VAL	4.7
2	H	247	PRO	4.7
1	B	108	LEU	4.7
1	B	699	LYS	4.7
1	A	80	PHE	4.7
1	B	364	TYR	4.7
1	B	253	ASP	4.6
2	H	381	ILE	4.6
1	B	149	GLY	4.6
2	H	329	VAL	4.6
4	F	54	ALA	4.6
2	H	20	PHE	4.6
1	A	742	ALA	4.6
1	A	746	THR	4.6
1	A	89	GLY	4.6
2	H	361	GLU	4.6
1	B	203	PHE	4.6
1	A	352	LEU	4.6
2	H	104	GLU	4.6

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Mol	Chain	Res	Type	RSRZ
2	H	380	LEU	4.6
1	B	515	SER	4.6
1	B	235	VAL	4.6
1	B	639	ILE	4.6
2	H	260	LYS	4.6
1	A	307	VAL	4.5
1	B	173	THR	4.5
1	A	574	VAL	4.5
1	A	221	LEU	4.5
2	H	23	LEU	4.5
1	A	90	VAL	4.5
1	A	242	ARG	4.5
4	F	40	SER	4.5
1	A	658	VAL	4.5
1	B	155	ASN	4.5
2	H	335	GLU	4.5
1	B	365	GLU	4.4
1	A	546	MET	4.4
2	H	85	ILE	4.4
1	B	256	THR	4.4
2	H	360	LEU	4.4
1	B	237	ALA	4.4
1	B	645	ARG	4.4
1	A	219	THR	4.4
1	A	88	GLY	4.3
2	H	103	GLU	4.3
1	B	194	GLU	4.3
2	H	400	ALA	4.3
4	F	12	ILE	4.3
2	G	105	GLY	4.3
1	A	342	GLY	4.3
1	B	79	MET	4.2
2	H	395	PHE	4.2
2	H	382	PRO	4.2
2	G	258	GLY	4.2
2	G	214	GLY	4.2
4	F	30	GLY	4.2
1	B	168	TYR	4.2
1	A	743	TYR	4.2
1	B	130	ASN	4.2
1	B	126	VAL	4.2
1	A	774	PHE	4.2

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Mol	Chain	Res	Type	RSRZ
2	G	397	GLY	4.2
1	A	339	ALA	4.2
1	B	322	ARG	4.2
2	G	108	GLY	4.2
2	H	201	VAL	4.1
1	A	391	THR	4.1
1	A	530	GLY	4.1
2	H	339	ASN	4.1
1	B	703	PHE	4.1
1	A	239	ALA	4.1
1	B	167	ALA	4.1
1	A	659	ASP	4.1
2	H	404	VAL	4.1
1	B	206	ILE	4.1
2	H	245	GLN	4.1
1	A	96	ASN	4.1
2	H	84	SER	4.1
1	B	166	GLU	4.1
1	B	204	ALA	4.1
1	A	82	PHE	4.1
2	H	263	LEU	4.1
2	H	336	LEU	4.1
2	H	111	LYS	4.0
1	B	317	ASP	4.0
1	B	689	MET	4.0
1	A	576	ARG	4.0
2	H	396	GLY	4.0
4	F	34	GLY	4.0
2	G	421	LYS	4.0
2	H	402	ILE	4.0
1	B	195	GLN	4.0
1	B	685	LEU	4.0
2	G	422	LYS	4.0
1	A	15	THR	4.0
2	G	388	TRP	4.0
2	G	62	PHE	4.0
4	E	10	VAL	4.0
1	B	154	LEU	4.0
2	H	394	TYR	3.9
1	A	92	LEU	3.9
1	A	237	ALA	3.9
1	A	547	ARG	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	684	MET	3.9
4	F	42	PHE	3.9
2	H	102	LYS	3.9
2	H	244	ILE	3.9
2	G	141	PRO	3.9
1	B	153	GLY	3.9
1	A	340	LYS	3.9
1	A	313	VAL	3.8
1	A	6	ASN	3.8
1	A	8	MET	3.8
1	B	697	ASN	3.8
2	H	19	ILE	3.8
1	B	78	GLY	3.8
1	B	127	VAL	3.8
1	B	700	GLU	3.8
1	A	94	ASP	3.8
2	G	275	ILE	3.8
2	G	257	ALA	3.7
1	B	240	PHE	3.7
1	A	664	THR	3.7
1	A	615	PHE	3.7
1	B	128	THR	3.7
1	A	84	VAL	3.7
1	A	548	ARG	3.7
2	H	386	SER	3.7
2	H	274	PRO	3.6
1	A	7	LYS	3.6
1	B	368	ALA	3.6
2	H	399	THR	3.6
2	H	397	GLY	3.6
1	B	646	GLU	3.6
2	G	140	SER	3.6
2	G	424	LYS	3.6
4	F	43	GLY	3.6
4	F	29	VAL	3.6
1	A	314	VAL	3.6
1	B	688	ILE	3.5
2	G	60	ASP	3.5
1	B	260	GLN	3.5
1	B	366	LYS	3.5
2	H	106	ASP	3.5
1	A	91	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	308	VAL	3.5
1	B	637	ARG	3.5
4	F	70	SER	3.5
2	H	346	PHE	3.5
2	H	359	TYR	3.5
1	B	257	LYS	3.4
2	G	426	TYR	3.4
1	B	172	ILE	3.4
1	B	308	VAL	3.4
4	E	72	ILE	3.4
2	H	337	ALA	3.4
1	B	692	ILE	3.4
1	B	175	SER	3.4
4	F	68	LEU	3.4
1	B	161	LYS	3.4
1	B	693	ILE	3.4
1	A	668	GLU	3.4
1	A	646	GLU	3.3
1	B	644	PRO	3.3
2	G	142	LYS	3.3
1	A	14	ARG	3.3
2	H	356	THR	3.3
1	B	513	HIS	3.3
1	A	390	VAL	3.3
1	A	101	LYS	3.3
2	G	387	VAL	3.2
4	F	69	LEU	3.2
1	A	389	VAL	3.2
2	G	396	GLY	3.2
1	A	392	ILE	3.2
2	H	393	PHE	3.2
1	A	238	ASN	3.2
2	H	105	GLY	3.2
2	H	353	GLY	3.2
2	H	109	ARG	3.1
1	B	162	ASP	3.1
1	B	741	ARG	3.1
2	H	110	TYR	3.1
1	A	667	ASP	3.1
1	B	512	ARG	3.1
2	H	243	PRO	3.1
1	B	640	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	396	ARG	3.1
1	B	638	ALA	3.1
2	H	22	LEU	3.0
1	A	105	GLY	3.0
2	H	385	ILE	3.0
1	A	549	PHE	3.0
2	G	386	SER	2.9
2	H	338	GLU	2.9
1	A	398	VAL	2.9
2	H	107	TYR	2.9
2	G	59	TYR	2.9
1	B	316	VAL	2.9
1	B	241	VAL	2.8
1	B	643	THR	2.8
1	A	393	PRO	2.8
2	G	274	PRO	2.8
1	A	622	ASN	2.8
1	B	160	SER	2.8
1	A	663	THR	2.8
2	H	330	LEU	2.8
1	A	665	TYR	2.7
2	H	355	ASP	2.7
1	B	205	VAL	2.7
1	A	575	SER	2.7
1	B	152	VAL	2.7
2	H	18	PHE	2.7
2	H	403	VAL	2.7
1	A	13	LYS	2.6
1	A	616	GLU	2.6
1	A	241	VAL	2.6
1	B	301	GLN	2.6
2	G	392	PRO	2.6
1	A	397	PRO	2.5
1	B	169	ALA	2.5
1	B	80	PHE	2.5
1	A	102	THR	2.4
1	A	240	PHE	2.4
1	A	10	ASP	2.4
1	A	394	THR	2.4
2	H	421	LYS	2.4
4	F	10	VAL	2.4
1	B	641	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	11	PRO	2.3
2	G	213	ILE	2.3
1	B	303	ASP	2.3
1	B	151	THR	2.3
1	B	124	VAL	2.2
2	G	425	SER	2.2
1	B	307	VAL	2.2
2	H	383	ILE	2.2
1	B	642	TYR	2.2
1	A	9	PHE	2.2
2	G	394	TYR	2.2
2	H	354	GLN	2.2
1	A	12	THR	2.2
1	B	171	ASP	2.1
1	A	617	VAL	2.1
1	B	170	ALA	2.1
1	A	619	ASP	2.1
1	A	621	GLU	2.1
1	B	258	ALA	2.1
4	F	72	ILE	2.0
1	A	395	ASN	2.0
1	A	103	GLY	2.0

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

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

## 6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

## 6.4 Ligands (i)

There are no ligands in this entry.

## 6.5 Other polymers (i)

There are no such residues in this entry.