



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 09:31 AM GMT

PDB ID : 3B5Y
Title : Crystal Structure of MsbA from Salmonella typhimurium with AMPPNP
Authors : Ward, A.; Reyes, C.L.; Yu, J.; Roth, C.B.; Chang, G.
Deposited on : 2007-10-26
Resolution : 4.50 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

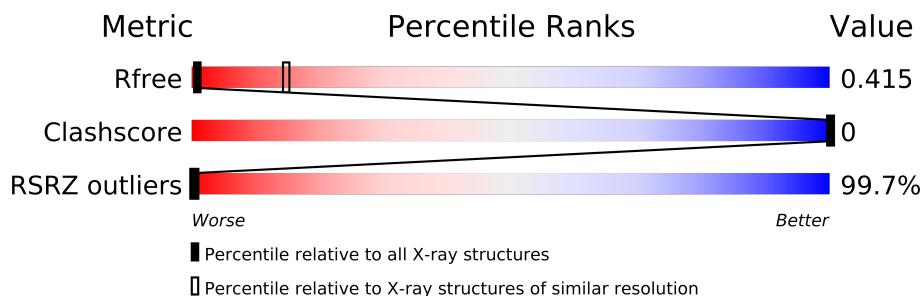
The following versions of software and data (see [references](#)) were used in the production of this report:

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





The reported resolution of this entry is 4.50 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	1029 (5.50-3.50)
Clashscore	79885	1300 (5.50-3.50)
RSRZ outliers	66119	1028 (5.50-3.50)

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 ≥ 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.

Mol	Chain	Length	Quality of chain
1	A	582	
1	B	582	
1	C	582	
1	D	582	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	ANP	A	5002	-	X
2	ANP	B	5001	-	X
2	ANP	C	5004	-	X
2	ANP	D	5003	-	X

2 Entry composition i

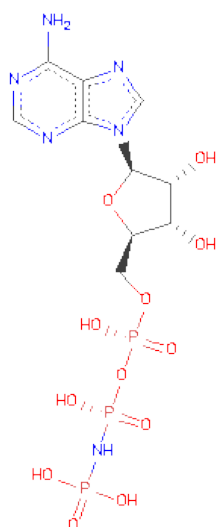
There are 2 unique types of molecules in this entry. The entry contains 2412 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Lipid A export ATP-binding/permease protein msbA.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
1	A	572	Total	C	0	0	572
			572	572			
1	B	572	Total	C	0	0	572
			572	572			
1	C	572	Total	C	0	0	572
			572	572			
1	D	572	Total	C	0	0	572
			572	572			

- Molecule 2 is PHOSPHOAMINOPHOSPHONICACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

Continued on next page...

Continued from previous page...

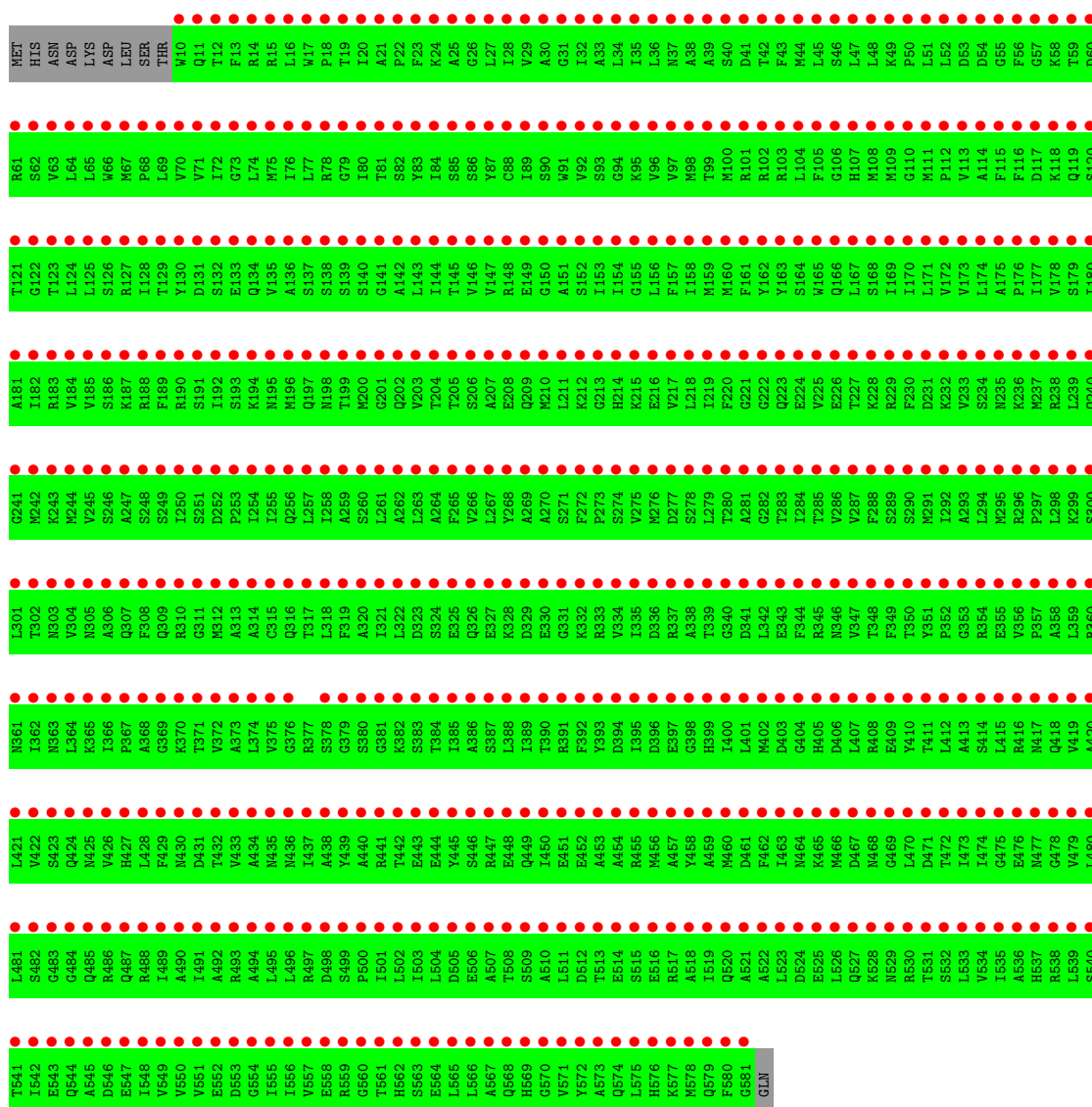
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

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: Lipid A export ATP-binding/permease protein msbA

Chain A: 



- Molecule 1: Lipid A export ATP-binding/permease protein msbA

Chain B: 

A181	T121	H61	MET
A182	G122	S62	ASN
A183	L123	V63	ASP
A184	L124	L64	LVS
B185	L125	L65	ASP
B186	S126	H66	LEU
A187	A127	H67	THR
A188	I128	P68	
F189	T129	L69	
R190	V130	V70	
S191	D131	V71	
L192	S132	L72	
S193	E133	G73	
K194	Q134	L74	
N195	V135	M75	
M196	A136	L76	
Q197	S137	L77	
N198	S138	H78	
T199	S139	G79	
M200	S140	L80	
G201	G141	T81	
Q202	A142	S82	
V203	L143	H83	
T204	L144	L84	
T205	L145	S85	
S206	V146	S86	
E207	V147	H87	
E208	R148	C88	
Q209	E149	L89	
M210	G150	S90	
L211	A151	H91	
K212	S152	V92	
G213	L153	S93	
H214	L154	O94	
K215	G155	K95	
E216	L156	V96	
V217	F157	V97	
L218	L158	H98	
L219	M159	T99	
M220	M160	M100	
G221	F161	E101	
G222	V162	L102	
Q223	V163	L103	
E224	S164	L104	
V225	M165	F105	
E226	Q166	G106	
T227	L167	H107	
K228	S168	M108	
R229	L169	M109	
F230	L170	G110	
D231	L171	M111	
K232	V172	P112	
V233	V173	V113	
S234	L174	A114	
K235	A175	F115	
K236	P176	F116	
M237	L177	L117	
R238	V178	K118	
L239	S179	O119	
T240	F180	L120	



L481	S482	G483	G484	Q485	R486	Q487	R488	I489	A490	I491	A492	R493	A494	L495	L496	R497	D498	S499	P500	I501	L502	I503	L504	D505	E506	A507	T508	S509	A510	L511	D512	T513	E514	S515	E516	R517	A518	I519	Q520	A521	A522	L523	D524	E525	L526	Q527	K528	N529	R530	T531	S532	L533	V534	I535	A536	H537	R538	L539	S540																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
T541	I542	E543	Q544	A545	D546	E547	I548	V549	V550	V551	E552	D553	G554	I555	I556	V557	E558	R559	G560	T561	H562	S563	E564	I565	L566	A567	Q568	H569	G570	V571	Y572	A573	Q574	L575	H576	K577	K578	Q579	F580	G581	Gln																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	262.93Å 121.24Å 173.12Å 90.00° 121.89° 90.00°	Depositor
Resolution (Å)	19.98 – 4.50 19.98 – 4.50	Depositor EDS
% Data completeness (in resolution range)	94.9 (19.98-4.50) 95.0 (19.98-4.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 4.54Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.295 , 0.343 0.402 , 0.415	Depositor DCC
R_{free} test set	2602 reflections (10.04%)	DCC
Wilson B-factor (Å ²)	184.2	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.86 , -10.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 25959 reflections	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	2412	wwPDB-VP
Average B, all atoms (Å ²)	219.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ANP

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	$\# Z > 5$

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 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	572	0	0	0	0
1	B	572	0	0	0	0
1	C	572	0	0	0	0
1	D	572	0	0	0	0
2	A	31	0	13	0	0
2	B	31	0	13	0	0
2	C	31	0	13	0	0
2	D	31	0	13	0	0
All	All	2412	0	52	0	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 0.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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

5.3.2 Protein sidechains ⓘ

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

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

4 ligands are modelled in this entry.

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	ANP	A	5002	-	33,33,33	1.55	5 (15%)	51,52,52	2.08	9 (17%)
2	ANP	B	5001	-	33,33,33	2.79	12 (36%)	51,52,52	2.64	12 (23%)
2	ANP	C	5004	-	33,33,33	1.59	5 (15%)	51,52,52	2.08	9 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ANP	D	5003	-	33,33,33	1.58	5 (15%)	51,52,52	2.08	10 (19%)

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	ANP	A	5002	-	-	0/18/38/38	0/1/3/3
2	ANP	B	5001	-	-	0/18/38/38	0/1/3/3
2	ANP	C	5004	-	-	0/18/38/38	0/1/3/3
2	ANP	D	5003	-	-	0/18/38/38	0/1/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	5001	ANP	PB-O1B	-6.20	1.38	1.46
2	B	5001	ANP	PB-N3B	6.07	1.69	1.64
2	B	5001	ANP	C4-N9	5.61	1.45	1.37
2	B	5001	ANP	PG-N3B	5.00	1.68	1.64
2	B	5001	ANP	C8-N9	4.48	1.43	1.36
2	B	5001	ANP	PA-O3A	4.29	1.67	1.59
2	B	5001	ANP	PA-O1A	-4.24	1.35	1.51
2	C	5004	ANP	PB-N3B	3.72	1.67	1.64
2	D	5003	ANP	PG-N3B	3.69	1.67	1.64
2	D	5003	ANP	PB-N3B	3.66	1.67	1.64
2	C	5004	ANP	PG-N3B	3.56	1.67	1.64
2	B	5001	ANP	PB-O2B	-3.53	1.44	1.55
2	A	5002	ANP	PG-N3B	3.51	1.67	1.64
2	A	5002	ANP	PB-N3B	3.50	1.67	1.64
2	B	5001	ANP	C3'-C4'	-3.24	1.44	1.53
2	C	5004	ANP	PB-O2B	-3.11	1.46	1.55
2	A	5002	ANP	PB-O2B	-3.06	1.46	1.55
2	D	5003	ANP	PB-O2B	-3.04	1.46	1.55
2	B	5001	ANP	O3'-C3'	3.01	1.50	1.43
2	B	5001	ANP	O4'-C1'	-2.98	1.36	1.41
2	C	5004	ANP	PG-O2G	-2.79	1.47	1.55
2	D	5003	ANP	PG-O2G	-2.76	1.47	1.55
2	A	5002	ANP	PG-O2G	-2.75	1.47	1.55
2	D	5003	ANP	C4-N9	2.42	1.41	1.37
2	C	5004	ANP	C4-N9	2.33	1.41	1.37
2	A	5002	ANP	C4-N9	2.30	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	5001	ANP	C1'-N9	2.21	1.55	1.48

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	5001	ANP	C4'-O4'-C1'	-9.43	99.50	109.75
2	B	5001	ANP	C8-N9-C4	-8.27	100.58	106.90
2	B	5001	ANP	O4'-C1'-C2'	-6.70	96.50	106.77
2	C	5004	ANP	O4'-C1'-C2'	-6.26	97.18	106.77
2	A	5002	ANP	O4'-C1'-C2'	-6.22	97.24	106.77
2	D	5003	ANP	C4'-O4'-C1'	-6.22	102.99	109.75
2	D	5003	ANP	O4'-C1'-C2'	-6.22	97.24	106.77
2	A	5002	ANP	C4'-O4'-C1'	-6.18	103.04	109.75
2	C	5004	ANP	C4'-O4'-C1'	-6.15	103.07	109.75
2	B	5001	ANP	C4-C5-N7	5.34	114.10	109.52
2	C	5004	ANP	C8-N9-C4	-4.64	103.36	106.90
2	A	5002	ANP	C8-N9-C4	-4.62	103.37	106.90
2	C	5004	ANP	O1B-PB-N3B	-4.61	104.87	111.83
2	D	5003	ANP	C8-N9-C4	-4.59	103.39	106.90
2	A	5002	ANP	O1B-PB-N3B	-4.57	104.92	111.83
2	D	5003	ANP	O1B-PB-N3B	-4.56	104.94	111.83
2	B	5001	ANP	O2B-PB-O1B	4.48	120.24	109.89
2	A	5002	ANP	C2'-C1'-N9	4.45	124.70	113.27
2	D	5003	ANP	C2'-C1'-N9	4.44	124.67	113.27
2	C	5004	ANP	C2'-C1'-N9	4.37	124.49	113.27
2	C	5004	ANP	O1G-PG-N3B	-4.29	105.34	111.83
2	A	5002	ANP	O1G-PG-N3B	-4.27	105.37	111.83
2	D	5003	ANP	O1G-PG-N3B	-4.27	105.38	111.83
2	B	5001	ANP	C2'-C1'-N9	4.18	123.99	113.27
2	B	5001	ANP	O1B-PB-N3B	-3.96	105.85	111.83
2	C	5004	ANP	O2B-PB-O1B	3.40	117.74	109.89
2	D	5003	ANP	O2B-PB-O1B	3.40	117.74	109.89
2	A	5002	ANP	O2B-PB-O1B	3.37	117.67	109.89
2	B	5001	ANP	C1'-N9-C4	3.29	132.33	126.64
2	B	5001	ANP	PB-N3B-PG	-3.16	124.75	130.07
2	D	5003	ANP	C4-C5-N7	3.02	112.11	109.52
2	B	5001	ANP	O3G-PG-O1G	-2.92	106.10	113.60
2	C	5004	ANP	C4-C5-N7	2.86	111.97	109.52
2	A	5002	ANP	C4-C5-N7	2.77	111.89	109.52
2	B	5001	ANP	O2'-C2'-C1'	-2.52	103.61	111.23
2	D	5003	ANP	O3G-PG-O2G	2.38	114.47	107.66
2	C	5004	ANP	O3G-PG-O2G	2.37	114.46	107.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	5002	ANP	O3G-PG-O2G	2.35	114.41	107.66
2	B	5001	ANP	C3'-C2'-C1'	-2.14	97.56	100.91
2	D	5003	ANP	PB-N3B-PG	-2.01	126.68	130.07

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

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

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	572/582 (98%)	28.06	571 (99%) 0 0	142, 225, 277, 312	0
1	B	572/582 (98%)	28.73	570 (99%) 0 0	112, 212, 274, 321	0
1	C	572/582 (98%)	28.92	571 (99%) 0 0	130, 218, 271, 309	0
1	D	572/582 (98%)	31.66	570 (99%) 0 0	132, 220, 271, 314	0
All	All	2288/2328 (98%)	29.34	2282 (99%) 0 0	112, 219, 274, 321	0

All (2282) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	530	ARG	148.7
1	C	49	LYS	145.2
1	B	562	HIS	141.2
1	D	320	ALA	139.2
1	C	345	ARG	135.8
1	B	406	ASP	133.2
1	D	558	GLU	129.6
1	D	321	ILE	128.9
1	A	562	HIS	122.4
1	D	297	PRO	118.0
1	D	296	ARG	112.8
1	B	558	GLU	110.0
1	D	170	ILE	109.5
1	B	568	GLN	103.7
1	C	131	ASP	101.4
1	B	569	HIS	100.6
1	B	517	ARG	99.7
1	D	572	TYR	98.8
1	A	151	ALA	97.8
1	D	41	ASP	97.3
1	C	48	LEU	96.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	302	THR	95.9
1	C	111	MET	95.6
1	C	364	LEU	94.6
1	D	298	LEU	92.8
1	C	564	GLU	92.1
1	A	73	GLY	91.5
1	D	171	LEU	91.5
1	C	253	PRO	91.1
1	C	531	THR	90.3
1	C	45	LEU	90.1
1	D	259	ALA	90.0
1	B	171	LEU	89.7
1	B	296	ARG	88.0
1	A	317	THR	87.9
1	D	369	GLY	87.5
1	B	303	ASN	85.4
1	A	43	PHE	85.3
1	B	563	SER	84.8
1	D	168	SER	84.5
1	C	578	MET	84.0
1	B	323	ASP	83.8
1	C	64	LEU	83.8
1	B	343	GLU	83.5
1	C	471	ASP	83.3
1	D	169	ILE	82.5
1	D	426	VAL	82.2
1	D	167	LEU	81.6
1	B	444	GLU	81.3
1	D	476	GLU	81.3
1	D	464	ASN	81.1
1	D	326	GLN	81.1
1	D	577	LYS	80.7
1	C	577	LYS	80.4
1	B	346	ASN	80.3
1	C	75	MET	80.1
1	B	276	MET	80.1
1	A	19	THR	79.5
1	B	363	ASN	79.3
1	D	197	GLN	79.2
1	C	173	VAL	78.9
1	B	348	THR	78.2
1	D	548	ILE	78.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	460	MET	77.8
1	D	303	ASN	77.8
1	D	525	GLU	77.4
1	D	228	LYS	77.3
1	B	304	VAL	76.9
1	C	180	ILE	76.9
1	D	149	GLU	76.6
1	C	397	GLU	76.6
1	A	320	ALA	76.5
1	B	102	ARG	76.4
1	C	134	GLN	76.3
1	A	514	GLU	76.0
1	C	333	ARG	75.8
1	D	239	LEU	75.4
1	A	545	ALA	74.8
1	D	323	ASP	74.5
1	B	324	SER	74.2
1	D	42	THR	74.0
1	D	75	MET	73.8
1	C	187	LYS	73.7
1	D	166	GLN	73.3
1	C	455	ARG	73.1
1	B	427	HIS	72.6
1	C	186	SER	72.2
1	D	364	LEU	71.9
1	A	568	GLN	71.5
1	A	262	ALA	71.4
1	A	476	GLU	70.8
1	C	183	ARG	70.8
1	A	176	PRO	70.8
1	C	396	ASP	70.7
1	A	517	ARG	70.6
1	A	76	ILE	70.5
1	A	240	GLN	70.1
1	B	335	ILE	69.9
1	D	47	LEU	69.9
1	D	35	ILE	69.6
1	A	72	ILE	69.5
1	D	567	ALA	68.3
1	A	166	GLN	68.0
1	C	346	ASN	67.8
1	B	183	ARG	67.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	238	ARG	67.5
1	B	325	GLU	67.3
1	A	576	HIS	66.7
1	C	159	MET	66.6
1	B	184	VAL	66.5
1	C	19	THR	66.4
1	C	326	GLN	66.4
1	D	437	ILE	66.3
1	C	412	LEU	66.2
1	D	363	ASN	66.1
1	A	172	VAL	65.8
1	B	145	THR	65.6
1	A	557	VAL	65.5
1	D	46	SER	65.5
1	A	256	GLN	65.4
1	D	216	GLU	65.1
1	A	253	PRO	65.0
1	D	471	ASP	64.9
1	D	329	ASP	64.9
1	A	183	ARG	64.9
1	B	401	LEU	64.8
1	D	452	GLU	64.6
1	A	411	THR	64.5
1	B	111	MET	64.5
1	A	98	MET	64.2
1	D	333	ARG	64.2
1	D	21	ALA	64.0
1	B	297	PRO	63.9
1	B	578	MET	63.8
1	C	264	ALA	63.8
1	C	363	ASN	63.3
1	B	133	GLU	63.2
1	A	241	GLY	63.1
1	C	177	ILE	63.0
1	A	449	GLN	62.8
1	D	258	ILE	62.5
1	C	304	VAL	62.4
1	C	365	LYS	62.3
1	D	544	GLN	62.1
1	A	35	ILE	62.0
1	B	218	LEU	62.0
1	D	18	PRO	61.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	577	LYS	61.7
1	D	159	MET	61.5
1	D	150	GLY	61.4
1	A	153	ILE	61.4
1	D	50	PRO	61.3
1	A	111	MET	61.2
1	A	46	SER	61.1
1	A	455	ARG	61.0
1	C	219	ILE	61.0
1	D	110	GLY	60.9
1	A	150	GLY	60.7
1	D	432	THR	60.6
1	C	408	ARG	60.2
1	A	561	THR	60.0
1	D	573	ALA	60.0
1	A	394	ASP	60.0
1	B	443	GLU	59.8
1	D	155	GLY	59.7
1	B	473	ILE	59.3
1	B	134	GLN	59.2
1	A	303	ASN	59.2
1	D	446	SER	59.2
1	A	245	VAL	58.8
1	B	32	ILE	58.7
1	C	571	VAL	58.7
1	B	272	PHE	58.7
1	C	335	ILE	58.6
1	B	410	TYR	58.6
1	A	184	VAL	58.4
1	C	79	GLY	58.4
1	C	158	ILE	58.3
1	D	72	ILE	58.1
1	A	281	ALA	58.0
1	C	325	GLU	58.0
1	D	343	GLU	57.9
1	A	194	LYS	57.8
1	D	36	LEU	57.6
1	C	407	LEU	57.5
1	A	414	SER	57.3
1	B	476	GLU	57.3
1	D	322	LEU	57.1
1	A	244	MET	57.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	76	ILE	56.9
1	C	522	ALA	56.7
1	A	189	PHE	56.7
1	D	391	ARG	56.7
1	B	42	THR	56.6
1	D	194	LYS	56.6
1	B	447	ARG	56.4
1	D	142	ALA	56.4
1	B	344	PHE	56.3
1	A	530	ARG	56.3
1	A	578	MET	56.3
1	A	363	ASN	56.1
1	D	152	SER	56.1
1	C	574	GLN	55.9
1	D	524	ASP	55.8
1	B	173	VAL	55.6
1	A	175	ALA	55.5
1	A	556	ILE	55.4
1	D	133	GLU	55.3
1	C	108	MET	54.9
1	C	77	LEU	54.8
1	A	341	ASP	54.7
1	D	436	ASN	54.6
1	D	336	ASP	54.6
1	B	520	GLN	54.5
1	D	413	ALA	54.3
1	D	447	ARG	54.3
1	D	335	ILE	54.3
1	B	232	LYS	54.2
1	D	568	GLN	54.1
1	D	29	VAL	54.0
1	D	232	LYS	54.0
1	D	191	SER	54.0
1	A	145	THR	54.0
1	C	237	MET	53.9
1	D	520	GLN	53.9
1	D	444	GLU	53.7
1	D	517	ARG	53.7
1	C	432	THR	53.7
1	C	530	ARG	53.7
1	B	570	GLY	53.6
1	A	237	MET	53.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	493	ARG	53.3
1	C	256	GLN	53.3
1	B	300	SER	53.3
1	B	430	ASN	53.2
1	A	32	ILE	53.2
1	B	107	HIS	53.2
1	A	103	ARG	53.1
1	A	252	ASP	53.1
1	C	42	THR	53.1
1	A	182	ILE	53.0
1	A	477	ASN	52.9
1	A	415	LEU	52.9
1	B	345	ARG	52.8
1	D	557	VAL	52.8
1	A	261	LEU	52.8
1	A	340	GLY	52.8
1	A	102	ARG	52.7
1	D	337	ARG	52.7
1	A	369	GLY	52.7
1	C	291	MET	52.4
1	B	44	MET	52.4
1	B	529	ASN	52.3
1	D	180	ILE	52.3
1	D	201	GLY	52.1
1	D	455	ARG	52.0
1	B	557	VAL	51.9
1	D	261	LEU	51.8
1	C	368	ALA	51.8
1	D	44	MET	51.8
1	B	521	ALA	51.7
1	A	113	VAL	51.7
1	B	541	THR	51.6
1	B	158	ILE	51.5
1	B	409	GLU	51.3
1	B	326	GLN	51.3
1	B	432	THR	51.1
1	B	123	THR	51.1
1	A	228	LYS	51.0
1	C	52	LEU	51.0
1	D	19	THR	50.9
1	C	533	LEU	50.8
1	D	368	ALA	50.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	543	GLU	50.8
1	B	31	GLY	50.8
1	C	68	PRO	50.8
1	C	123	THR	50.7
1	B	186	SER	50.7
1	D	521	ALA	50.6
1	C	362	ILE	50.6
1	B	455	ARG	50.5
1	C	165	TRP	50.4
1	B	321	ILE	50.4
1	A	21	ALA	50.3
1	D	222	GLY	50.3
1	C	224	GLU	50.2
1	B	514	GLU	50.2
1	A	53	ASP	50.2
1	C	262	ALA	50.1
1	B	421	LEU	50.1
1	B	75	MET	50.0
1	A	212	LYS	50.0
1	A	422	VAL	49.7
1	B	439	TYR	49.6
1	A	471	ASP	49.6
1	B	95	LYS	49.6
1	D	397	GLU	49.6
1	A	112	PRO	49.5
1	A	443	GLU	49.4
1	B	69	LEU	49.4
1	C	516	GLU	49.4
1	B	36	LEU	49.3
1	B	275	VAL	49.1
1	C	517	ARG	49.1
1	A	558	GLU	49.0
1	A	325	GLU	48.8
1	C	107	HIS	48.8
1	C	50	PRO	48.7
1	A	518	ALA	48.7
1	B	216	GLU	48.6
1	A	298	LEU	48.6
1	D	317	THR	48.4
1	D	11	GLN	48.4
1	C	261	LEU	48.3
1	D	24	LYS	48.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	525	GLU	48.3
1	D	526	LEU	48.2
1	A	365	LYS	48.2
1	C	130	TYR	48.0
1	A	52	LEU	48.0
1	C	176	PRO	47.9
1	D	443	GLU	47.9
1	C	297	PRO	47.9
1	C	227	THR	47.7
1	D	529	ASN	47.7
1	D	48	LEU	47.6
1	B	301	LEU	47.5
1	A	318	LEU	47.4
1	B	513	THR	47.4
1	C	518	ALA	47.4
1	B	52	LEU	47.3
1	D	473	ILE	47.2
1	B	280	THR	47.1
1	C	344	PHE	47.1
1	B	331	GLY	47.0
1	B	312	MET	47.0
1	A	49	LYS	47.0
1	D	361	ASN	46.9
1	D	281	ALA	46.8
1	D	143	LEU	46.8
1	B	17	TRP	46.8
1	B	576	HIS	46.7
1	C	103	ARG	46.7
1	B	180	ILE	46.7
1	D	185	VAL	46.6
1	D	215	LYS	46.6
1	A	138	SER	46.6
1	A	242	MET	46.6
1	C	302	THR	46.5
1	A	572	TYR	46.4
1	C	529	ASN	46.4
1	A	326	GLN	46.4
1	C	296	ARG	46.4
1	D	99	THR	46.3
1	B	362	ILE	46.3
1	D	28	ILE	46.2
1	C	431	ASP	46.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	395	ILE	46.1
1	C	133	GLU	46.1
1	D	576	HIS	46.0
1	D	563	SER	45.9
1	D	341	ASP	45.9
1	A	180	ILE	45.8
1	B	228	LYS	45.7
1	C	154	ILE	45.7
1	A	104	LEU	45.7
1	C	330	GLU	45.7
1	B	579	GLN	45.5
1	D	559	ARG	45.5
1	B	172	VAL	45.4
1	C	528	LYS	45.4
1	D	578	MET	45.4
1	C	439	TYR	45.4
1	A	195	ASN	45.4
1	D	146	VAL	45.3
1	A	217	VAL	45.2
1	D	181	ALA	45.2
1	A	213	GLY	45.2
1	C	327	GLU	45.2
1	B	396	ASP	45.1
1	A	28	ILE	45.1
1	D	503	ILE	45.1
1	C	125	LEU	45.1
1	A	432	THR	45.0
1	D	313	ALA	45.0
1	A	77	LEU	45.0
1	A	393	TYR	44.9
1	D	539	LEU	44.8
1	D	45	LEU	44.7
1	B	215	LYS	44.7
1	C	401	LEU	44.7
1	A	188	ARG	44.7
1	D	173	VAL	44.6
1	D	220	PHE	44.5
1	B	155	GLY	44.4
1	B	431	ASP	44.4
1	C	202	GLN	44.3
1	D	490	ALA	44.3
1	B	361	ASN	44.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	352	PRO	44.3
1	A	581	GLY	44.3
1	D	111	MET	44.2
1	A	36	LEU	44.2
1	C	443	GLU	44.1
1	A	435	ASN	44.1
1	A	580	PHE	44.1
1	A	502	LEU	44.0
1	C	570	GLY	43.9
1	D	108	MET	43.9
1	B	295	MET	43.9
1	C	178	VAL	43.9
1	B	299	LYS	43.8
1	C	307	GLN	43.8
1	D	566	LEU	43.8
1	A	314	ALA	43.8
1	C	413	ALA	43.7
1	B	98	MET	43.6
1	B	62	SER	43.6
1	B	130	TYR	43.5
1	A	364	LEU	43.5
1	C	171	LEU	43.5
1	D	257	LEU	43.5
1	B	19	THR	43.5
1	C	559	ARG	43.4
1	D	69	LEU	43.4
1	B	328	LYS	43.3
1	C	453	ALA	43.3
1	B	310	ARG	43.3
1	D	51	LEU	43.3
1	B	450	ILE	43.2
1	C	236	LYS	43.1
1	C	477	ASN	43.1
1	C	162	TYR	43.1
1	B	445	TYR	43.1
1	C	160	MET	43.1
1	D	17	TRP	43.1
1	D	459	ALA	43.0
1	B	371	THR	43.0
1	A	564	GLU	43.0
1	B	566	LEU	42.9
1	D	183	ARG	42.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	318	LEU	42.8
1	A	268	TYR	42.8
1	D	502	LEU	42.8
1	C	470	LEU	42.7
1	B	540	SER	42.7
1	C	151	ALA	42.6
1	D	370	LYS	42.5
1	B	76	ILE	42.4
1	A	460	MET	42.4
1	D	137	SER	42.3
1	A	276	MET	42.2
1	C	515	SER	42.2
1	B	477	ASN	42.2
1	C	69	LEU	42.2
1	A	292	ILE	42.1
1	C	562	HIS	42.1
1	A	348	THR	42.1
1	A	235	ASN	42.0
1	D	130	TYR	42.0
1	C	329	ASP	42.0
1	A	248	SER	41.9
1	D	187	LYS	41.9
1	A	69	LEU	41.8
1	A	523	LEU	41.7
1	A	101	ARG	41.7
1	B	397	GLU	41.7
1	B	472	THR	41.7
1	D	20	ILE	41.6
1	D	410	TYR	41.6
1	D	138	SER	41.6
1	D	396	ASP	41.6
1	D	175	ALA	41.5
1	B	306	ALA	41.5
1	B	74	LEU	41.5
1	C	472	THR	41.5
1	C	569	HIS	41.5
1	A	520	GLN	41.4
1	B	92	VAL	41.4
1	D	227	THR	41.4
1	D	224	GLU	41.4
1	D	295	MET	41.3
1	A	426	VAL	41.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	422	VAL	41.3
1	C	421	LEU	41.2
1	C	235	ASN	41.1
1	D	104	LEU	41.0
1	D	218	LEU	41.0
1	B	341	ASP	40.9
1	D	574	GLN	40.9
1	B	544	GLN	40.9
1	C	54	ASP	40.9
1	B	156	LEU	40.8
1	B	399	HIS	40.8
1	C	521	ALA	40.7
1	B	71	VAL	40.7
1	A	174	LEU	40.7
1	A	454	ALA	40.7
1	A	79	GLY	40.7
1	D	58	LYS	40.7
1	B	113	VAL	40.6
1	B	198	ASN	40.6
1	A	78	ARG	40.6
1	B	451	GLU	40.6
1	B	53	ASP	40.5
1	C	58	LYS	40.5
1	A	470	LEU	40.5
1	D	49	LYS	40.4
1	C	182	ILE	40.4
1	C	46	SER	40.3
1	D	475	GLY	40.3
1	D	199	THR	40.2
1	A	239	LEU	40.2
1	C	191	SER	40.2
1	A	329	ASP	40.1
1	A	300	SER	40.1
1	D	83	TYR	40.0
1	D	165	TRP	40.0
1	A	154	ILE	40.0
1	B	35	ILE	40.0
1	B	106	GLY	39.9
1	D	15	ARG	39.8
1	B	307	GLN	39.8
1	A	521	ALA	39.8
1	A	80	ILE	39.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	260	SER	39.7
1	C	25	ALA	39.6
1	D	71	VAL	39.6
1	C	369	GLY	39.6
1	D	229	ARG	39.6
1	B	547	GLU	39.5
1	D	182	ILE	39.5
1	B	101	ARG	39.4
1	D	278	SER	39.4
1	A	191	SER	39.4
1	B	368	ALA	39.4
1	D	186	SER	39.4
1	B	177	ILE	39.4
1	B	503	ILE	39.3
1	B	43	PHE	39.3
1	B	564	GLU	39.3
1	A	392	PHE	39.2
1	B	370	LYS	39.2
1	C	266	VAL	39.1
1	D	22	PRO	39.1
1	B	154	ILE	39.1
1	C	78	ARG	39.0
1	A	579	GLN	39.0
1	A	405	HIS	39.0
1	B	575	LEU	39.0
1	C	263	LEU	38.9
1	C	96	VAL	38.8
1	A	171	LEU	38.8
1	C	323	ASP	38.8
1	B	446	SER	38.8
1	D	236	LYS	38.8
1	B	282	GLY	38.7
1	D	541	THR	38.7
1	C	305	ASN	38.7
1	C	67	MET	38.7
1	A	573	ALA	38.7
1	B	257	LEU	38.6
1	C	210	MET	38.6
1	B	523	LEU	38.6
1	A	187	LYS	38.6
1	C	22	PRO	38.5
1	A	64	LEU	38.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	104	LEU	38.5
1	D	26	GLY	38.5
1	A	566	LEU	38.5
1	A	529	ASN	38.4
1	D	302	THR	38.4
1	B	398	GLY	38.4
1	B	471	ASP	38.3
1	C	563	SER	38.3
1	A	453	ALA	38.3
1	A	567	ALA	38.2
1	C	557	VAL	38.2
1	C	519	ILE	38.1
1	A	148	ARG	38.1
1	A	198	ASN	38.1
1	A	263	LEU	38.1
1	C	170	ILE	38.0
1	A	224	GLU	38.0
1	A	330	GLU	38.0
1	A	149	GLU	38.0
1	B	49	LYS	38.0
1	C	473	ILE	38.0
1	D	367	PRO	38.0
1	B	22	PRO	38.0
1	A	65	LEU	38.0
1	D	556	ILE	37.9
1	B	72	ILE	37.9
1	D	102	ARG	37.9
1	C	16	LEU	37.9
1	A	18	PRO	37.9
1	A	165	TRP	37.7
1	B	461	ASP	37.7
1	B	124	LEU	37.7
1	D	144	ILE	37.6
1	A	327	GLU	37.6
1	C	334	VAL	37.6
1	C	245	VAL	37.6
1	D	371	THR	37.5
1	D	325	GLU	37.5
1	D	282	GLY	37.5
1	A	275	VAL	37.4
1	C	281	ALA	37.4
1	D	393	TYR	37.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	417	ASN	37.4
1	B	138	SER	37.3
1	B	73	GLY	37.3
1	D	477	ASN	37.3
1	B	571	VAL	37.3
1	C	150	GLY	37.3
1	D	163	TYR	37.3
1	D	43	PHE	37.2
1	D	103	ARG	37.2
1	B	89	ILE	37.2
1	C	122	GLY	37.1
1	C	579	GLN	37.1
1	B	572	TYR	37.1
1	D	40	SER	37.1
1	D	531	THR	37.1
1	D	10	TRP	37.1
1	C	155	GLY	37.0
1	A	134	GLN	37.0
1	D	32	ILE	36.9
1	D	445	TYR	36.9
1	B	131	ASP	36.9
1	D	562	HIS	36.9
1	C	312	MET	36.9
1	A	515	SER	36.8
1	C	573	ALA	36.8
1	A	229	ARG	36.8
1	A	297	PRO	36.7
1	A	468	ASN	36.7
1	B	146	VAL	36.7
1	C	205	THR	36.6
1	B	223	GLN	36.6
1	B	233	VAL	36.6
1	A	216	GLU	36.6
1	C	21	ALA	36.6
1	D	348	THR	36.6
1	D	431	ASP	36.6
1	D	283	THR	36.5
1	A	361	ASN	36.5
1	C	525	GLU	36.5
1	D	56	PHE	36.5
1	A	577	LYS	36.5
1	A	301	LEU	36.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	182	ILE	36.4
1	A	83	TYR	36.4
1	A	234	SER	36.3
1	C	415	LEU	36.3
1	D	516	GLU	36.3
1	A	140	SER	36.2
1	B	220	PHE	36.2
1	D	439	TYR	36.2
1	C	572	TYR	36.2
1	D	307	GLN	36.1
1	B	222	GLY	36.1
1	D	401	LEU	36.1
1	C	539	LEU	36.0
1	B	277	ASP	36.0
1	C	353	GLY	35.9
1	D	154	ILE	35.9
1	D	392	PHE	35.9
1	D	238	ARG	35.9
1	D	134	GLN	35.9
1	C	43	PHE	35.9
1	D	174	LEU	35.9
1	D	210	MET	35.9
1	B	574	GLN	35.9
1	A	368	ALA	35.8
1	D	311	GLY	35.8
1	B	212	LYS	35.8
1	D	205	THR	35.8
1	B	336	ASP	35.8
1	C	336	ASP	35.7
1	B	149	GLU	35.7
1	C	568	GLN	35.7
1	C	169	ILE	35.7
1	D	202	GLN	35.7
1	A	238	ARG	35.6
1	C	391	ARG	35.6
1	B	237	MET	35.6
1	B	20	ILE	35.6
1	D	247	ALA	35.6
1	C	456	MET	35.6
1	B	68	PRO	35.5
1	C	188	ARG	35.5
1	A	143	LEU	35.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	232	LYS	35.5
1	B	34	LEU	35.5
1	A	458	TYR	35.4
1	C	168	SER	35.4
1	A	39	ALA	35.4
1	B	502	LEU	35.3
1	D	330	GLU	35.3
1	C	175	ALA	35.3
1	C	276	MET	35.3
1	C	500	PRO	35.3
1	C	153	ILE	35.2
1	A	227	THR	35.2
1	A	452	GLU	35.2
1	D	293	ALA	35.2
1	B	395	ILE	35.1
1	A	223	GLN	35.1
1	C	343	GLU	35.1
1	D	53	ASP	35.1
1	C	208	GLU	35.1
1	B	448	GLU	35.0
1	A	27	LEU	35.0
1	D	190	ARG	35.0
1	C	254	ILE	34.9
1	D	402	MET	34.7
1	C	17	TRP	34.7
1	C	15	ARG	34.7
1	D	148	ARG	34.7
1	C	145	THR	34.7
1	C	26	GLY	34.7
1	B	28	ILE	34.7
1	A	255	ILE	34.6
1	B	227	THR	34.6
1	D	285	THR	34.6
1	A	225	VAL	34.6
1	D	453	ALA	34.6
1	A	328	LYS	34.5
1	C	447	ARG	34.5
1	A	135	VAL	34.5
1	B	340	GLY	34.4
1	A	61	ARG	34.4
1	D	472	THR	34.4
1	A	370	LYS	34.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	242	MET	34.4
1	C	24	LYS	34.3
1	A	247	ALA	34.3
1	C	361	ASN	34.3
1	A	106	GLY	34.3
1	C	300	SER	34.2
1	A	427	HIS	34.1
1	C	576	HIS	34.1
1	A	542	ILE	34.0
1	C	73	GLY	33.9
1	B	188	ARG	33.9
1	B	236	LYS	33.9
1	B	187	LYS	33.8
1	A	118	LYS	33.8
1	A	492	ALA	33.8
1	B	322	LEU	33.7
1	D	268	TYR	33.6
1	A	409	GLU	33.6
1	D	244	MET	33.6
1	A	141	GLY	33.6
1	C	249	SER	33.6
1	B	332	LYS	33.6
1	C	20	ILE	33.6
1	D	442	THR	33.6
1	C	468	ASN	33.5
1	A	490	ALA	33.5
1	A	475	GLY	33.5
1	B	93	SER	33.5
1	A	214	HIS	33.5
1	A	560	GLY	33.5
1	C	152	SER	33.4
1	D	344	PHE	33.4
1	C	464	ASN	33.4
1	B	39	ALA	33.3
1	C	394	ASP	33.3
1	D	153	ILE	33.3
1	A	322	LEU	33.3
1	C	435	ASN	33.3
1	B	231	ASP	33.2
1	C	546	ASP	33.2
1	C	102	ARG	33.2
1	A	418	GLN	33.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	448	GLU	33.1
1	D	411	THR	33.1
1	D	427	HIS	33.1
1	A	565	LEU	33.0
1	C	299	LYS	33.0
1	B	365	LYS	33.0
1	D	493	ARG	32.9
1	A	205	THR	32.9
1	C	250	ILE	32.9
1	C	184	VAL	32.8
1	C	149	GLU	32.8
1	C	400	ILE	32.8
1	C	194	LYS	32.8
1	A	181	ALA	32.8
1	C	57	GLY	32.8
1	A	360	ARG	32.8
1	C	321	ILE	32.8
1	C	451	GLU	32.8
1	D	346	ASN	32.8
1	B	329	ASP	32.8
1	B	565	LEU	32.8
1	C	161	PHE	32.7
1	C	430	ASN	32.7
1	B	224	GLU	32.7
1	C	41	ASP	32.6
1	A	410	TYR	32.5
1	C	34	LEU	32.5
1	B	99	THR	32.5
1	C	419	VAL	32.5
1	C	278	SER	32.5
1	D	62	SER	32.5
1	D	52	LEU	32.5
1	C	460	MET	32.5
1	B	419	VAL	32.4
1	A	323	ASP	32.4
1	A	119	GLN	32.4
1	C	164	SER	32.3
1	C	31	GLY	32.3
1	C	558	GLU	32.3
1	D	195	ASN	32.2
1	B	452	GLU	32.1
1	C	80	ILE	32.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	394	ASP	32.0
1	D	57	GLY	31.9
1	B	141	GLY	31.9
1	D	16	LEU	31.9
1	A	304	VAL	31.9
1	D	421	LEU	31.8
1	C	74	LEU	31.8
1	C	121	THR	31.8
1	D	122	GLY	31.8
1	B	369	GLY	31.8
1	D	237	MET	31.8
1	A	310	ARG	31.8
1	B	440	ALA	31.7
1	A	524	ASP	31.7
1	B	561	THR	31.7
1	A	100	MET	31.6
1	D	504	LEU	31.6
1	A	71	VAL	31.6
1	D	219	ILE	31.5
1	D	200	MET	31.5
1	C	179	SER	31.4
1	C	513	THR	31.4
1	B	528	LYS	31.4
1	B	119	GLN	31.4
1	A	541	THR	31.4
1	C	115	PHE	31.4
1	A	421	LEU	31.4
1	A	406	ASP	31.3
1	B	80	ILE	31.3
1	C	476	GLU	31.3
1	C	367	PRO	31.3
1	B	422	VAL	31.3
1	B	14	ARG	31.2
1	A	494	ALA	31.2
1	D	360	ARG	31.2
1	C	127	ARG	31.2
1	C	354	ARG	31.2
1	C	29	VAL	31.1
1	B	79	GLY	31.1
1	B	78	ARG	31.1
1	A	51	LEU	31.1
1	B	559	ARG	31.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	277	ASP	31.1
1	C	228	LYS	31.0
1	D	280	THR	31.0
1	C	70	VAL	31.0
1	D	100	MET	31.0
1	C	523	LEU	31.0
1	B	169	ILE	30.9
1	C	72	ILE	30.9
1	B	531	THR	30.9
1	C	225	VAL	30.8
1	B	241	GLY	30.8
1	D	39	ALA	30.8
1	C	402	MET	30.8
1	C	32	ILE	30.7
1	C	454	ALA	30.7
1	D	394	ASP	30.6
1	B	12	THR	30.6
1	C	503	ILE	30.6
1	B	94	GLY	30.6
1	D	119	GLN	30.6
1	B	127	ARG	30.5
1	B	516	GLU	30.5
1	A	464	ASN	30.4
1	D	569	HIS	30.4
1	B	46	SER	30.4
1	D	547	GLU	30.3
1	D	125	LEU	30.3
1	D	223	GLN	30.3
1	C	124	LEU	30.3
1	A	294	LEU	30.3
1	A	156	LEU	30.3
1	B	122	GLY	30.3
1	A	444	GLU	30.2
1	B	283	THR	30.2
1	D	37	ASN	30.1
1	C	514	GLU	30.1
1	A	94	GLY	30.1
1	A	179	SER	30.1
1	A	543	GLU	30.1
1	D	63	VAL	30.0
1	C	405	HIS	30.0
1	D	233	VAL	30.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	119	GLN	30.0
1	A	259	ALA	30.0
1	D	221	GLY	29.9
1	A	342	LEU	29.9
1	C	141	GLY	29.9
1	A	243	LYS	29.9
1	D	492	ALA	29.9
1	A	167	LEU	29.9
1	B	526	LEU	29.8
1	A	226	GLU	29.8
1	B	508	THR	29.8
1	A	220	PHE	29.7
1	B	137	SER	29.7
1	D	564	GLU	29.7
1	D	13	PHE	29.7
1	A	403	ASP	29.6
1	C	452	GLU	29.6
1	A	68	PRO	29.6
1	C	109	MET	29.6
1	D	300	SER	29.5
1	B	250	ILE	29.5
1	A	108	MET	29.5
1	D	79	GLY	29.4
1	A	569	HIS	29.2
1	D	419	VAL	29.2
1	A	302	THR	29.1
1	D	497	ARG	29.1
1	C	565	LEU	29.1
1	A	434	ALA	29.0
1	B	151	ALA	29.0
1	A	163	TYR	29.0
1	B	144	ILE	29.0
1	B	548	ILE	28.9
1	D	496	LEU	28.9
1	C	328	LYS	28.9
1	D	458	TYR	28.9
1	A	197	GLN	28.8
1	C	30	ALA	28.8
1	C	242	MET	28.7
1	B	103	ARG	28.7
1	A	400	ILE	28.7
1	B	314	ALA	28.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	353	GLY	28.7
1	A	157	PHE	28.7
1	C	71	VAL	28.6
1	B	546	ASP	28.6
1	D	501	ILE	28.6
1	C	190	ARG	28.6
1	B	405	HIS	28.6
1	B	178	VAL	28.5
1	A	127	ARG	28.5
1	B	247	ALA	28.5
1	A	513	THR	28.5
1	D	465	LYS	28.5
1	B	45	LEU	28.5
1	C	100	MET	28.5
1	A	571	VAL	28.4
1	D	491	ILE	28.4
1	C	541	THR	28.4
1	B	573	ALA	28.4
1	C	174	LEU	28.3
1	D	33	ALA	28.3
1	A	295	MET	28.3
1	C	156	LEU	28.3
1	A	82	SER	28.3
1	D	31	GLY	28.2
1	D	118	LYS	28.2
1	C	185	VAL	28.2
1	D	279	LEU	28.2
1	A	346	ASN	28.2
1	D	301	LEU	28.2
1	A	442	THR	28.2
1	D	65	LEU	28.1
1	A	123	THR	28.0
1	A	438	ALA	28.0
1	C	437	ILE	28.0
1	A	222	GLY	28.0
1	D	84	ILE	28.0
1	A	496	LEU	28.0
1	D	251	SER	27.9
1	D	408	ARG	27.9
1	B	132	SER	27.9
1	D	366	ILE	27.9
1	D	542	ILE	27.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	258	ILE	27.9
1	A	74	LEU	27.9
1	B	47	LEU	27.9
1	B	414	SER	27.8
1	A	75	MET	27.8
1	D	95	LYS	27.8
1	D	212	LYS	27.7
1	A	190	ARG	27.7
1	C	404	GLY	27.7
1	C	283	THR	27.7
1	C	279	LEU	27.7
1	D	304	VAL	27.6
1	D	193	SER	27.5
1	B	214	HIS	27.5
1	C	341	ASP	27.5
1	D	461	ASP	27.5
1	A	371	THR	27.5
1	A	575	LEU	27.5
1	A	121	THR	27.4
1	D	253	PRO	27.4
1	A	401	LEU	27.4
1	D	131	ASP	27.3
1	C	265	PHE	27.3
1	C	214	HIS	27.3
1	B	311	GLY	27.3
1	A	218	LEU	27.2
1	D	204	THR	27.2
1	C	13	PHE	27.2
1	B	428	LEU	27.1
1	D	449	GLN	27.1
1	A	271	SER	27.1
1	B	453	ALA	27.1
1	C	248	SER	27.0
1	B	185	VAL	27.0
1	D	211	LEU	27.0
1	D	435	ASN	27.0
1	C	520	GLN	27.0
1	D	324	SER	26.9
1	B	23	PHE	26.9
1	B	372	VAL	26.9
1	D	124	LEU	26.9
1	B	334	VAL	26.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	204	THR	26.8
1	D	440	ALA	26.8
1	B	338	ALA	26.8
1	B	515	SER	26.8
1	B	337	ARG	26.8
1	A	451	GLU	26.7
1	D	334	VAL	26.7
1	D	12	THR	26.7
1	D	581	GLY	26.7
1	D	189	PHE	26.6
1	C	309	GLN	26.6
1	B	391	ARG	26.6
1	C	53	ASP	26.6
1	A	278	SER	26.5
1	D	434	ALA	26.5
1	C	395	ILE	26.5
1	B	465	LYS	26.5
1	B	77	LEU	26.5
1	B	97	VAL	26.4
1	C	370	LYS	26.4
1	D	127	ARG	26.4
1	D	269	ALA	26.4
1	B	298	LEU	26.3
1	B	140	SER	26.2
1	A	291	MET	26.2
1	C	306	ALA	26.2
1	D	495	LEU	26.2
1	D	156	LEU	26.1
1	A	20	ILE	26.1
1	B	201	GLY	26.1
1	C	317	THR	26.1
1	C	411	THR	26.1
1	A	210	MET	26.0
1	A	528	LYS	26.0
1	A	257	LEU	26.0
1	D	409	GLU	26.0
1	D	217	VAL	26.0
1	B	500	PRO	26.0
1	B	21	ALA	26.0
1	D	407	LEU	26.0
1	B	402	MET	25.9
1	D	294	LEU	25.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	567	ALA	25.8
1	C	56	PHE	25.8
1	A	177	ILE	25.7
1	D	54	ASP	25.7
1	B	253	PRO	25.7
1	B	205	THR	25.7
1	B	327	GLU	25.7
1	D	312	MET	25.7
1	C	409	GLU	25.6
1	B	400	ILE	25.6
1	A	539	LEU	25.6
1	D	248	SER	25.6
1	B	333	ARG	25.5
1	A	503	ILE	25.4
1	B	152	SER	25.4
1	A	311	GLY	25.4
1	D	123	THR	25.4
1	A	196	MET	25.3
1	D	274	SER	25.3
1	B	109	MET	25.3
1	D	277	ASP	25.3
1	B	136	ALA	25.3
1	C	18	PRO	25.2
1	D	209	GLN	25.2
1	C	167	LEU	25.2
1	B	309	GLN	25.1
1	D	113	VAL	25.1
1	A	24	LYS	25.1
1	B	142	ALA	25.0
1	B	518	ALA	25.0
1	C	222	GLY	25.0
1	D	575	LEU	25.0
1	B	105	PHE	25.0
1	C	44	MET	24.9
1	C	491	ILE	24.9
1	C	410	TYR	24.9
1	A	173	VAL	24.9
1	C	293	ALA	24.9
1	D	92	VAL	24.9
1	D	177	ILE	24.9
1	B	519	ILE	24.9
1	C	392	PHE	24.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	280	THR	24.9
1	C	251	SER	24.9
1	A	41	ASP	24.8
1	B	308	PHE	24.8
1	B	292	ILE	24.8
1	C	148	ARG	24.8
1	B	366	ILE	24.8
1	C	142	ALA	24.8
1	A	306	ALA	24.8
1	D	25	ALA	24.8
1	A	37	ASN	24.7
1	D	225	VAL	24.7
1	C	313	ALA	24.7
1	C	257	LEU	24.7
1	B	33	ALA	24.6
1	C	372	VAL	24.6
1	A	473	ILE	24.6
1	B	61	ARG	24.6
1	C	247	ALA	24.5
1	B	342	LEU	24.5
1	B	263	LEU	24.5
1	C	580	PHE	24.5
1	C	501	ILE	24.5
1	A	92	VAL	24.5
1	A	522	ALA	24.5
1	C	246	SER	24.4
1	C	218	LEU	24.4
1	C	467	ASP	24.4
1	D	109	MET	24.4
1	A	202	GLN	24.4
1	C	538	ARG	24.4
1	B	90	SER	24.4
1	B	467	ASP	24.3
1	A	48	LEU	24.3
1	D	286	VAL	24.3
1	C	442	THR	24.2
1	B	40	SER	24.2
1	C	469	GLY	24.2
1	D	340	GLY	24.2
1	A	209	GLN	24.2
1	C	55	GLY	24.2
1	D	70	VAL	24.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	141	GLY	24.1
1	B	242	MET	24.1
1	A	472	THR	24.1
1	D	518	ALA	24.1
1	C	506	GLU	24.1
1	D	273	PRO	24.1
1	B	468	ASN	24.1
1	D	430	ASN	24.1
1	B	294	LEU	24.1
1	D	117	ASP	24.1
1	D	105	PHE	24.1
1	A	199	THR	24.1
1	A	33	ALA	24.1
1	D	101	ARG	24.1
1	A	335	ILE	24.0
1	B	271	SER	24.0
1	B	64	LEU	24.0
1	A	168	SER	24.0
1	B	464	ASN	24.0
1	D	500	PRO	24.0
1	C	436	ASN	24.0
1	A	38	ALA	23.9
1	C	418	GLN	23.9
1	A	211	LEU	23.9
1	A	299	LYS	23.9
1	D	214	HIS	23.9
1	B	239	LEU	23.8
1	C	458	TYR	23.8
1	A	413	ALA	23.8
1	B	251	SER	23.8
1	A	249	SER	23.8
1	C	147	VAL	23.8
1	A	412	LEU	23.7
1	B	279	LEU	23.7
1	B	202	GLN	23.7
1	B	339	THR	23.7
1	D	179	SER	23.6
1	D	68	PRO	23.6
1	A	142	ALA	23.6
1	D	77	LEU	23.6
1	D	342	LEU	23.6
1	C	196	MET	23.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	438	ALA	23.5
1	B	25	ALA	23.5
1	C	414	SER	23.5
1	A	531	THR	23.5
1	A	548	ILE	23.5
1	A	467	ASP	23.5
1	C	298	LEU	23.5
1	C	544	GLN	23.5
1	A	164	SER	23.4
1	C	290	SER	23.3
1	A	114	ALA	23.3
1	A	44	MET	23.3
1	B	190	ARG	23.2
1	D	275	VAL	23.2
1	B	225	VAL	23.2
1	C	129	THR	23.2
1	C	295	MET	23.2
1	D	107	HIS	23.2
1	B	83	TYR	23.2
1	D	290	SER	23.2
1	D	74	LEU	23.1
1	D	488	ARG	23.1
1	D	78	ARG	23.1
1	D	241	GLY	23.1
1	A	372	VAL	23.1
1	B	221	GLY	23.1
1	B	125	LEU	23.0
1	D	365	LYS	23.0
1	D	287	VAL	23.0
1	D	467	ASP	23.0
1	A	516	GLU	23.0
1	C	189	PHE	23.0
1	D	468	ASN	23.0
1	C	28	ILE	23.0
1	D	522	ALA	23.0
1	C	446	SER	22.9
1	C	14	ARG	22.9
1	A	186	SER	22.9
1	D	549	VAL	22.9
1	D	88	CYS	22.9
1	A	501	ILE	22.9
1	C	403	ASP	22.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	30	ALA	22.9
1	A	152	SER	22.9
1	C	390	THR	22.8
1	C	277	ASP	22.8
1	B	437	ILE	22.8
1	C	239	LEU	22.8
1	A	332	LYS	22.8
1	B	501	ILE	22.8
1	C	494	ALA	22.8
1	B	367	PRO	22.8
1	A	116	PHE	22.7
1	B	238	ARG	22.7
1	B	175	ALA	22.7
1	A	367	PRO	22.7
1	C	211	LEU	22.7
1	D	23	PHE	22.7
1	D	487	GLN	22.6
1	D	262	ALA	22.6
1	C	398	GLY	22.6
1	A	105	PHE	22.6
1	B	65	LEU	22.6
1	B	273	PRO	22.5
1	C	33	ALA	22.5
1	D	76	ILE	22.5
1	C	65	LEU	22.5
1	C	504	LEU	22.5
1	A	526	LEU	22.5
1	D	145	THR	22.5
1	A	23	PHE	22.4
1	C	371	THR	22.4
1	D	347	VAL	22.4
1	C	89	ILE	22.4
1	A	147	VAL	22.4
1	D	160	MET	22.4
1	C	112	PRO	22.3
1	D	265	PHE	22.3
1	A	307	GLN	22.3
1	C	220	PHE	22.3
1	B	320	ALA	22.3
1	A	126	SER	22.3
1	A	30	ALA	22.3
1	D	580	PHE	22.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	136	ALA	22.2
1	A	308	PHE	22.2
1	B	26	GLY	22.2
1	B	166	GLN	22.2
1	C	204	THR	22.2
1	B	256	GLN	22.2
1	B	415	LEU	22.2
1	C	303	ASN	22.2
1	A	136	ALA	22.2
1	A	489	ILE	22.2
1	C	294	LEU	22.2
1	D	533	LEU	22.2
1	C	36	LEU	22.2
1	B	229	ARG	22.2
1	D	489	ILE	22.2
1	B	168	SER	22.1
1	C	331	GLY	22.1
1	C	213	GLY	22.1
1	D	545	ALA	22.1
1	D	372	VAL	22.1
1	D	428	LEU	22.0
1	B	441	ARG	22.0
1	D	245	VAL	22.0
1	A	279	LEU	22.0
1	C	280	THR	22.0
1	C	23	PHE	22.0
1	C	27	LEU	22.0
1	B	210	MET	22.0
1	B	81	THR	21.9
1	C	35	ILE	21.9
1	B	330	GLU	21.9
1	A	50	PRO	21.9
1	D	64	LEU	21.9
1	B	360	ARG	21.8
1	B	170	ILE	21.8
1	A	115	PHE	21.8
1	D	115	PHE	21.8
1	B	70	VAL	21.8
1	B	84	ILE	21.8
1	B	265	PHE	21.7
1	C	434	ALA	21.7
1	B	524	ASP	21.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	188	ARG	21.6
1	A	441	ARG	21.6
1	C	192	ILE	21.6
1	B	494	ALA	21.6
1	D	270	ALA	21.6
1	B	408	ARG	21.6
1	A	201	GLY	21.6
1	D	192	ILE	21.6
1	C	37	ASN	21.5
1	A	120	SER	21.5
1	A	296	ARG	21.5
1	A	313	ALA	21.5
1	A	316	GLN	21.5
1	A	315	CYS	21.5
1	B	354	ARG	21.5
1	B	492	ALA	21.5
1	C	556	ILE	21.5
1	D	546	ASP	21.5
1	B	108	MET	21.4
1	A	389	ILE	21.4
1	A	221	GLY	21.4
1	A	144	ILE	21.3
1	B	139	SER	21.3
1	B	197	GLN	21.3
1	A	88	CYS	21.3
1	B	293	ALA	21.3
1	A	574	GLN	21.3
1	D	389	ILE	21.3
1	D	240	GLN	21.2
1	D	73	GLY	21.2
1	B	407	LEU	21.2
1	A	89	ILE	21.2
1	A	264	ALA	21.2
1	C	422	VAL	21.2
1	C	465	LYS	21.2
1	D	255	ILE	21.2
1	B	176	PRO	21.2
1	C	492	ALA	21.2
1	B	199	THR	21.2
1	A	95	LYS	21.2
1	A	117	ASP	21.1
1	C	448	GLU	21.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	364	LEU	21.1
1	B	456	MET	21.1
1	C	81	THR	21.1
1	D	14	ARG	21.1
1	C	308	PHE	21.0
1	C	91	TRP	21.0
1	D	208	GLU	21.0
1	A	232	LYS	21.0
1	C	146	VAL	21.0
1	C	226	GLU	20.9
1	D	203	VAL	20.9
1	D	513	THR	20.9
1	D	98	MET	20.9
1	B	18	PRO	20.9
1	C	527	GLN	20.9
1	C	275	VAL	20.9
1	C	114	ALA	20.8
1	A	506	GLU	20.8
1	A	158	ILE	20.8
1	C	110	GLY	20.8
1	C	215	LYS	20.8
1	C	138	SER	20.8
1	D	94	GLY	20.8
1	D	172	VAL	20.8
1	D	555	ILE	20.7
1	B	542	ILE	20.7
1	A	324	SER	20.7
1	C	581	GLY	20.7
1	D	196	MET	20.7
1	A	146	VAL	20.7
1	A	265	PHE	20.6
1	D	451	GLU	20.6
1	B	284	ILE	20.6
1	B	413	ALA	20.6
1	B	27	LEU	20.6
1	A	478	GLY	20.6
1	B	538	ARG	20.6
1	B	496	LEU	20.6
1	A	26	GLY	20.5
1	A	122	GLY	20.5
1	D	121	THR	20.5
1	A	66	TRP	20.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	178	VAL	20.5
1	D	106	GLY	20.5
1	D	514	GLU	20.4
1	A	208	GLU	20.4
1	C	63	VAL	20.4
1	B	258	ILE	20.3
1	B	359	LEU	20.3
1	B	181	ALA	20.3
1	C	526	LEU	20.3
1	C	524	ASP	20.3
1	A	436	ASN	20.3
1	B	522	ALA	20.3
1	C	316	GLN	20.3
1	D	507	ALA	20.3
1	C	85	SER	20.3
1	D	571	VAL	20.3
1	A	493	ARG	20.2
1	A	430	ASN	20.2
1	B	264	ALA	20.2
1	B	165	TRP	20.2
1	A	193	SER	20.2
1	A	423	SER	20.1
1	B	545	ALA	20.1
1	A	128	ILE	20.1
1	C	98	MET	20.1
1	A	507	ALA	20.1
1	C	566	LEU	20.1
1	C	195	ASN	20.1
1	D	260	SER	20.1
1	B	285	THR	20.0
1	B	29	VAL	20.0
1	D	120	SER	20.0
1	A	192	ILE	20.0
1	A	547	GLU	20.0
1	C	348	THR	20.0
1	C	498	ASP	20.0
1	A	137	SER	19.9
1	C	337	ARG	19.9
1	C	105	PHE	19.9
1	A	345	ARG	19.9
1	C	287	VAL	19.9
1	C	493	ARG	19.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	114	ALA	19.9
1	D	151	ALA	19.9
1	D	96	VAL	19.8
1	B	200	MET	19.8
1	C	252	ASP	19.8
1	C	282	GLY	19.8
1	A	555	ILE	19.8
1	C	120	SER	19.8
1	D	89	ILE	19.7
1	C	203	VAL	19.7
1	B	490	ALA	19.7
1	C	172	VAL	19.7
1	D	59	THR	19.6
1	D	139	SER	19.6
1	C	83	TYR	19.6
1	C	244	MET	19.6
1	C	212	LYS	19.6
1	B	189	PHE	19.6
1	A	544	GLN	19.6
1	D	331	GLY	19.6
1	B	507	ALA	19.6
1	D	27	LEU	19.6
1	C	324	SER	19.6
1	A	40	SER	19.5
1	C	311	GLY	19.5
1	A	170	ILE	19.5
1	D	157	PHE	19.5
1	B	211	LEU	19.5
1	D	523	LEU	19.5
1	D	362	ILE	19.5
1	B	194	LYS	19.5
1	C	229	ARG	19.5
1	B	167	LEU	19.5
1	D	454	ALA	19.5
1	B	162	TYR	19.4
1	C	449	GLN	19.4
1	C	206	SER	19.4
1	D	128	ILE	19.4
1	A	495	LEU	19.4
1	C	495	LEU	19.3
1	D	264	ALA	19.3
1	A	448	GLU	19.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	506	GLU	19.3
1	C	268	TYR	19.3
1	B	274	SER	19.3
1	C	548	ILE	19.3
1	D	498	ASP	19.3
1	A	42	THR	19.3
1	B	100	MET	19.3
1	B	442	THR	19.3
1	D	147	VAL	19.2
1	D	355	GLU	19.2
1	A	204	THR	19.2
1	B	315	CYS	19.2
1	C	87	TYR	19.2
1	C	101	ARG	19.2
1	A	559	ARG	19.1
1	B	317	THR	19.1
1	B	157	PHE	19.1
1	B	412	LEU	19.1
1	D	66	TRP	19.1
1	A	59	THR	19.1
1	B	318	LEU	19.0
1	A	58	LYS	19.0
1	A	230	PHE	19.0
1	B	56	PHE	19.0
1	D	226	GLU	19.0
1	A	107	HIS	19.0
1	C	271	SER	19.0
1	C	260	SER	18.9
1	A	34	LEU	18.9
1	A	129	THR	18.9
1	D	390	THR	18.9
1	B	66	TRP	18.9
1	B	434	ALA	18.8
1	B	234	SER	18.8
1	C	86	SER	18.8
1	A	31	GLY	18.8
1	B	41	ASP	18.8
1	D	86	SER	18.8
1	A	231	ASP	18.8
1	A	258	ILE	18.7
1	A	169	ILE	18.7
1	C	549	VAL	18.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	478	GLY	18.7
1	C	128	ILE	18.6
1	C	315	CYS	18.6
1	B	219	ILE	18.6
1	C	126	SER	18.5
1	C	444	GLU	18.5
1	B	533	LEU	18.5
1	C	423	SER	18.5
1	C	438	ALA	18.5
1	B	143	LEU	18.5
1	C	88	CYS	18.5
1	B	433	VAL	18.5
1	C	459	ALA	18.5
1	B	458	TYR	18.4
1	B	110	GLY	18.4
1	B	504	LEU	18.4
1	A	450	ILE	18.4
1	B	527	GLN	18.4
1	A	469	GLY	18.4
1	B	555	ILE	18.4
1	D	34	LEU	18.4
1	D	579	GLN	18.3
1	A	402	MET	18.3
1	A	99	THR	18.3
1	C	209	GLN	18.3
1	A	459	ALA	18.3
1	A	491	ILE	18.2
1	D	438	ALA	18.2
1	B	88	CYS	18.2
1	A	305	ASN	18.2
1	A	446	SER	18.2
1	B	196	MET	18.2
1	B	244	MET	18.2
1	B	248	SER	18.1
1	C	267	LEU	18.1
1	C	166	GLN	18.1
1	D	560	GLY	18.1
1	D	327	GLU	18.1
1	B	270	ALA	18.1
1	A	474	ILE	18.1
1	B	288	PHE	18.0
1	A	347	VAL	18.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	82	SER	18.0
1	D	527	GLN	18.0
1	A	286	VAL	18.0
1	D	250	ILE	18.0
1	A	233	VAL	18.0
1	B	13	PHE	18.0
1	C	66	TRP	18.0
1	B	11	GLN	18.0
1	A	333	ARG	17.9
1	A	395	ILE	17.9
1	B	230	PHE	17.9
1	D	532	SER	17.9
1	B	254	ILE	17.9
1	A	289	SER	17.8
1	A	407	LEU	17.8
1	D	412	LEU	17.7
1	D	469	GLY	17.7
1	C	113	VAL	17.7
1	C	502	LEU	17.7
1	A	200	MET	17.7
1	A	70	VAL	17.7
1	B	581	GLY	17.7
1	B	235	ASN	17.7
1	A	67	MET	17.6
1	C	12	THR	17.6
1	C	389	ILE	17.6
1	A	397	GLU	17.6
1	D	406	ASP	17.6
1	A	488	ARG	17.6
1	C	366	ILE	17.6
1	C	507	ALA	17.6
1	B	267	LEU	17.6
1	B	539	LEU	17.6
1	B	118	LYS	17.6
1	B	411	THR	17.5
1	B	495	LEU	17.5
1	D	178	VAL	17.5
1	C	259	ALA	17.5
1	B	128	ILE	17.5
1	D	534	VAL	17.5
1	B	63	VAL	17.5
1	B	353	GLY	17.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	243	LYS	17.5
1	B	115	PHE	17.5
1	C	199	THR	17.4
1	D	91	TRP	17.4
1	A	431	ASP	17.4
1	A	125	LEU	17.4
1	B	174	LEU	17.4
1	C	84	ILE	17.4
1	C	143	LEU	17.4
1	B	305	ASN	17.3
1	D	235	ASN	17.3
1	B	126	SER	17.3
1	D	456	MET	17.3
1	A	334	VAL	17.3
1	C	496	LEU	17.2
1	C	106	GLY	17.2
1	C	547	GLU	17.2
1	B	209	GLN	17.2
1	B	203	VAL	17.2
1	D	158	ILE	17.2
1	C	427	HIS	17.2
1	B	260	SER	17.2
1	B	436	ASN	17.2
1	C	99	THR	17.2
1	D	450	ILE	17.2
1	D	129	THR	17.2
1	C	373	ALA	17.2
1	D	306	ALA	17.2
1	B	120	SER	17.2
1	B	470	LEU	17.2
1	B	509	SER	17.1
1	D	234	SER	17.1
1	C	272	PHE	17.1
1	D	256	GLN	17.1
1	D	271	SER	17.1
1	B	150	GLY	17.1
1	C	320	ALA	17.1
1	B	153	ILE	17.0
1	A	533	LEU	17.0
1	A	465	LYS	17.0
1	B	389	ILE	17.0
1	D	161	PHE	17.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	433	VAL	17.0
1	B	226	GLU	17.0
1	B	16	LEU	17.0
1	D	506	GLU	16.9
1	C	355	GLU	16.9
1	C	59	THR	16.9
1	C	416	ARG	16.9
1	C	490	ALA	16.9
1	A	10	TRP	16.8
1	A	437	ILE	16.8
1	B	424	GLN	16.8
1	C	62	SER	16.8
1	A	428	LEU	16.8
1	D	310	ARG	16.7
1	C	322	LEU	16.7
1	B	291	MET	16.7
1	C	221	GLY	16.7
1	B	373	ALA	16.7
1	D	538	ARG	16.7
1	C	230	PHE	16.7
1	C	461	ASP	16.7
1	A	457	ALA	16.7
1	D	345	ARG	16.7
1	B	491	ILE	16.6
1	D	403	ASP	16.6
1	D	418	GLN	16.6
1	C	555	ILE	16.6
1	D	97	VAL	16.5
1	A	133	GLU	16.5
1	C	144	ILE	16.5
1	A	285	THR	16.5
1	B	121	THR	16.5
1	A	352	PRO	16.4
1	A	563	SER	16.4
1	C	542	ILE	16.4
1	D	231	ASP	16.4
1	A	236	LYS	16.4
1	D	116	PHE	16.4
1	C	118	LYS	16.4
1	C	457	ALA	16.3
1	C	92	VAL	16.3
1	A	272	PHE	16.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	499	SER	16.3
1	B	532	SER	16.3
1	C	463	ILE	16.3
1	A	284	ILE	16.3
1	A	504	LEU	16.2
1	C	95	LYS	16.2
1	A	505	ASP	16.2
1	A	497	ARG	16.2
1	D	478	GLY	16.2
1	B	96	VAL	16.2
1	B	449	GLN	16.2
1	C	532	SER	16.1
1	A	86	SER	16.1
1	A	440	ALA	16.1
1	C	301	LEU	16.1
1	C	163	TYR	16.0
1	C	207	ALA	16.0
1	A	273	PRO	16.0
1	C	561	THR	16.0
1	A	47	LEU	16.0
1	C	543	GLU	16.0
1	C	223	GLN	16.0
1	A	288	PHE	16.0
1	C	487	GLN	16.0
1	B	179	SER	15.9
1	A	445	TYR	15.9
1	A	337	ARG	15.9
1	A	290	SER	15.9
1	B	567	ALA	15.9
1	C	137	SER	15.9
1	B	48	LEU	15.8
1	B	159	MET	15.8
1	B	249	SER	15.8
1	A	331	GLY	15.8
1	D	318	LEU	15.8
1	D	38	ALA	15.8
1	B	435	ASN	15.8
1	A	391	ARG	15.8
1	C	339	THR	15.7
1	A	546	ASP	15.7
1	A	540	SER	15.6
1	B	499	SER	15.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	126	SER	15.6
1	B	351	TYR	15.6
1	C	90	SER	15.6
1	D	284	ILE	15.6
1	A	319	PHE	15.5
1	C	200	MET	15.5
1	C	537	HIS	15.5
1	B	278	SER	15.5
1	A	549	VAL	15.5
1	C	216	GLU	15.5
1	D	565	LEU	15.5
1	D	254	ILE	15.4
1	C	441	ARG	15.4
1	A	527	GLN	15.4
1	B	86	SER	15.4
1	D	164	SER	15.4
1	A	433	VAL	15.4
1	A	13	PHE	15.4
1	D	373	ALA	15.3
1	D	400	ILE	15.3
1	B	160	MET	15.3
1	A	343	GLU	15.3
1	D	55	GLY	15.3
1	D	494	ALA	15.3
1	D	414	SER	15.2
1	C	356	VAL	15.2
1	A	206	SER	15.2
1	D	184	VAL	15.2
1	A	336	ASP	15.1
1	C	399	HIS	15.1
1	B	15	ARG	15.1
1	D	550	VAL	15.1
1	B	543	GLU	15.1
1	C	197	GLN	15.0
1	C	545	ALA	15.0
1	B	262	ALA	15.0
1	D	230	PHE	15.0
1	B	10	TRP	15.0
1	D	90	SER	15.0
1	D	80	ILE	15.0
1	B	208	GLU	14.9
1	A	525	GLU	14.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	207	ALA	14.9
1	C	314	ALA	14.9
1	B	252	ASP	14.8
1	C	117	ASP	14.8
1	C	94	GLY	14.8
1	D	267	LEU	14.8
1	A	500	PRO	14.8
1	D	198	ASN	14.8
1	D	339	THR	14.7
1	A	25	ALA	14.7
1	D	207	ALA	14.7
1	B	469	GLY	14.7
1	A	90	SER	14.7
1	A	246	SER	14.7
1	A	93	SER	14.7
1	A	207	ALA	14.7
1	A	54	ASP	14.7
1	B	114	ALA	14.7
1	B	87	TYR	14.6
1	A	390	THR	14.6
1	D	162	TYR	14.6
1	B	489	ILE	14.6
1	D	425	ASN	14.5
1	B	425	ASN	14.5
1	B	454	ALA	14.5
1	C	450	ILE	14.4
1	B	129	THR	14.4
1	A	81	THR	14.4
1	D	81	THR	14.4
1	D	288	PHE	14.4
1	B	195	ASN	14.4
1	D	388	LEU	14.4
1	D	508	THR	14.3
1	B	213	GLY	14.3
1	C	234	SER	14.3
1	D	213	GLY	14.3
1	D	85	SER	14.2
1	A	124	LEU	14.2
1	A	267	LEU	14.2
1	D	82	SER	14.0
1	B	536	ALA	14.0
1	B	104	LEU	14.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	390	THR	14.0
1	A	282	GLY	14.0
1	A	159	MET	14.0
1	A	185	VAL	13.9
1	C	310	ARG	13.9
1	B	487	GLN	13.9
1	C	488	ARG	13.9
1	B	67	MET	13.9
1	A	139	SER	13.8
1	C	289	SER	13.8
1	C	136	ALA	13.8
1	B	266	VAL	13.8
1	C	47	LEU	13.7
1	C	61	ARG	13.7
1	A	110	GLY	13.7
1	B	290	SER	13.7
1	C	497	ARG	13.7
1	A	85	SER	13.7
1	B	530	ARG	13.6
1	C	359	LEU	13.6
1	D	316	GLN	13.6
1	D	441	ARG	13.6
1	C	139	SER	13.6
1	B	463	ILE	13.5
1	B	404	GLY	13.5
1	D	433	VAL	13.5
1	A	219	ILE	13.5
1	C	193	SER	13.5
1	A	309	GLN	13.4
1	C	286	VAL	13.4
1	D	132	SER	13.4
1	A	439	TYR	13.4
1	A	130	TYR	13.4
1	C	39	ALA	13.4
1	B	268	TYR	13.3
1	B	313	ALA	13.3
1	A	15	ARG	13.3
1	B	347	VAL	13.3
1	B	287	VAL	13.3
1	C	319	PHE	13.3
1	B	193	SER	13.3
1	C	360	ARG	13.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	96	VAL	13.2
1	D	305	ASN	13.2
1	C	231	ASP	13.2
1	C	489	ILE	13.2
1	A	499	SER	13.2
1	B	556	ILE	13.1
1	A	425	ASN	13.1
1	D	416	ARG	13.1
1	C	352	PRO	13.1
1	A	386	ALA	13.1
1	B	418	GLN	13.1
1	D	289	SER	13.0
1	C	425	ASN	12.9
1	D	206	SER	12.9
1	A	519	ILE	12.9
1	C	51	LEU	12.9
1	A	274	SER	12.9
1	B	417	ASN	12.9
1	B	161	PHE	12.8
1	B	550	VAL	12.8
1	B	245	VAL	12.8
1	D	272	PHE	12.8
1	A	534	VAL	12.8
1	A	456	MET	12.7
1	B	426	VAL	12.7
1	A	487	GLN	12.7
1	A	215	LYS	12.7
1	A	29	VAL	12.7
1	B	551	VAL	12.6
1	B	261	LEU	12.6
1	D	291	MET	12.6
1	A	84	ILE	12.6
1	D	356	VAL	12.6
1	D	552	GLU	12.6
1	A	14	ARG	12.6
1	D	417	ASN	12.6
1	A	552	GLU	12.6
1	D	315	CYS	12.6
1	D	505	ASP	12.6
1	C	475	GLY	12.5
1	A	254	ILE	12.5
1	D	292	ILE	12.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	355	GLU	12.5
1	B	281	ALA	12.5
1	D	387	SER	12.5
1	D	405	HIS	12.5
1	D	499	SER	12.5
1	A	553	ASP	12.5
1	C	417	ASN	12.5
1	A	429	PHE	12.5
1	A	480	LEU	12.5
1	A	131	ASP	12.4
1	D	528	LYS	12.4
1	B	460	MET	12.4
1	A	396	ASP	12.4
1	B	474	ILE	12.4
1	D	399	HIS	12.4
1	A	536	ALA	12.4
1	A	16	LEU	12.3
1	B	488	ARG	12.3
1	B	392	PHE	12.3
1	B	316	GLN	12.3
1	A	353	GLY	12.3
1	C	505	ASP	12.3
1	C	340	GLY	12.2
1	C	233	VAL	12.2
1	B	217	VAL	12.2
1	A	398	GLY	12.2
1	B	497	ARG	12.2
1	C	273	PRO	12.2
1	B	54	ASP	12.1
1	A	12	THR	12.1
1	D	140	SER	12.1
1	D	328	LYS	12.1
1	B	59	THR	12.1
1	B	393	TYR	12.1
1	C	181	ALA	12.1
1	D	561	THR	12.1
1	A	321	ILE	12.0
1	A	366	ILE	11.9
1	A	344	PHE	11.9
1	A	498	ASP	11.9
1	D	308	PHE	11.8
1	B	112	PRO	11.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	287	VAL	11.8
1	C	198	ASN	11.7
1	D	67	MET	11.7
1	A	293	ALA	11.7
1	B	240	GLN	11.7
1	B	135	VAL	11.7
1	A	62	SER	11.6
1	A	373	ALA	11.6
1	A	461	ASP	11.6
1	A	362	ILE	11.6
1	C	357	PRO	11.6
1	D	463	ILE	11.6
1	C	93	SER	11.5
1	A	419	VAL	11.5
1	C	550	VAL	11.5
1	A	266	VAL	11.5
1	A	466	MET	11.5
1	C	82	SER	11.4
1	B	423	SER	11.4
1	D	536	ALA	11.4
1	A	283	THR	11.4
1	A	91	TRP	11.4
1	D	357	PRO	11.4
1	B	459	ALA	11.3
1	D	309	GLN	11.3
1	D	266	VAL	11.3
1	B	374	LEU	11.3
1	D	470	LEU	11.3
1	A	349	PHE	11.3
1	A	551	VAL	11.3
1	B	319	PHE	11.2
1	C	11	GLN	11.2
1	D	474	ILE	11.2
1	C	534	VAL	11.2
1	C	284	ILE	11.2
1	C	536	ALA	11.1
1	C	462	PHE	11.1
1	A	109	MET	11.1
1	C	342	LEU	11.1
1	D	423	SER	11.1
1	A	203	VAL	11.0
1	C	116	PHE	11.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	534	VAL	11.0
1	B	91	TRP	10.9
1	A	63	VAL	10.9
1	D	93	SER	10.9
1	C	285	THR	10.9
1	B	24	LYS	10.9
1	D	512	ASP	10.9
1	B	259	ALA	10.9
1	D	87	TYR	10.9
1	A	87	TYR	10.8
1	A	447	ARG	10.8
1	B	357	PRO	10.8
1	A	388	LEU	10.7
1	D	354	ARG	10.7
1	B	403	ASP	10.7
1	B	51	LEU	10.7
1	C	540	SER	10.6
1	B	243	LYS	10.6
1	A	251	SER	10.6
1	A	60	ASP	10.6
1	B	191	SER	10.6
1	D	276	MET	10.6
1	C	347	VAL	10.6
1	C	201	GLY	10.6
1	B	560	GLY	10.6
1	B	60	ASP	10.6
1	C	388	LEU	10.6
1	B	387	SER	10.5
1	D	314	ALA	10.5
1	B	475	GLY	10.5
1	C	575	LEU	10.5
1	B	117	ASP	10.4
1	D	415	LEU	10.4
1	A	97	VAL	10.4
1	B	85	SER	10.3
1	D	515	SER	10.3
1	D	424	GLN	10.2
1	D	466	MET	10.2
1	B	549	VAL	10.2
1	A	22	PRO	10.2
1	D	319	PHE	10.1
1	B	37	ASN	10.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	478	GLY	10.0
1	C	157	PHE	10.0
1	A	161	PHE	10.0
1	B	457	ALA	10.0
1	A	374	LEU	10.0
1	C	255	ILE	10.0
1	C	241	GLY	10.0
1	C	374	LEU	10.0
1	B	416	ARG	9.9
1	A	387	SER	9.9
1	C	508	THR	9.9
1	A	463	ILE	9.8
1	A	312	MET	9.8
1	B	58	LYS	9.8
1	A	338	ALA	9.8
1	C	560	GLY	9.8
1	B	192	ILE	9.8
1	B	512	ASP	9.8
1	A	375	VAL	9.7
1	C	10	TRP	9.7
1	B	116	PHE	9.6
1	B	50	PRO	9.6
1	C	420	ALA	9.6
1	A	162	TYR	9.6
1	C	483	GLY	9.6
1	A	270	ALA	9.6
1	A	570	GLY	9.5
1	D	112	PRO	9.4
1	A	17	TRP	9.4
1	B	535	ILE	9.3
1	C	440	ALA	9.3
1	B	382	LYS	9.3
1	A	512	ASP	9.3
1	B	505	ASP	9.3
1	A	57	GLY	9.2
1	C	484	GLY	9.2
1	C	217	VAL	9.2
1	A	357	PRO	9.1
1	A	351	TYR	9.1
1	C	552	GLU	9.1
1	A	356	VAL	9.1
1	B	388	LEU	9.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	509	SER	8.9
1	B	510	ALA	8.9
1	D	551	VAL	8.9
1	A	408	ARG	8.9
1	C	97	VAL	8.9
1	C	288	PHE	8.9
1	C	424	GLN	8.8
1	B	349	PHE	8.8
1	C	510	ALA	8.8
1	D	299	LYS	8.8
1	A	382	LYS	8.7
1	A	508	THR	8.7
1	B	206	SER	8.6
1	C	240	GLN	8.6
1	D	519	ILE	8.6
1	C	243	LYS	8.6
1	C	428	LEU	8.6
1	C	292	ILE	8.6
1	D	383	SER	8.5
1	B	163	TYR	8.5
1	B	462	PHE	8.5
1	D	263	LEU	8.4
1	A	420	ALA	8.4
1	B	580	PHE	8.4
1	C	551	VAL	8.4
1	D	332	LYS	8.4
1	C	350	THR	8.3
1	A	11	GLN	8.3
1	D	176	PRO	8.3
1	B	383	SER	8.3
1	B	246	SER	8.3
1	C	40	SER	8.2
1	C	466	MET	8.2
1	D	338	ALA	8.2
1	A	399	HIS	8.1
1	B	350	THR	8.0
1	C	338	ALA	8.0
1	D	352	PRO	7.9
1	B	420	ALA	7.9
1	D	382	LYS	7.9
1	C	393	TYR	7.9
1	C	60	ASP	7.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	135	VAL	7.8
1	D	246	SER	7.8
1	C	535	ILE	7.8
1	D	351	TYR	7.8
1	D	249	SER	7.8
1	B	148	ARG	7.7
1	C	140	SER	7.7
1	A	339	THR	7.6
1	D	480	LEU	7.6
1	C	474	ILE	7.6
1	A	509	SER	7.6
1	A	160	MET	7.5
1	B	552	GLU	7.5
1	B	381	GLY	7.5
1	C	381	GLY	7.5
1	C	38	ALA	7.4
1	C	135	VAL	7.4
1	D	570	GLY	7.4
1	C	349	PHE	7.3
1	A	424	GLN	7.3
1	D	386	ALA	7.3
1	A	269	ALA	7.3
1	C	486	ARG	7.3
1	B	479	VAL	7.3
1	B	466	MET	7.2
1	C	554	GLY	7.2
1	A	359	LEU	7.1
1	D	349	PHE	7.0
1	D	30	ALA	6.9
1	A	383	SER	6.9
1	A	510	ALA	6.9
1	C	332	LYS	6.8
1	D	252	ASP	6.7
1	D	554	GLY	6.7
1	C	382	LYS	6.7
1	B	255	ILE	6.6
1	C	509	SER	6.6
1	D	553	ASP	6.6
1	D	535	ILE	6.5
1	C	406	ASP	6.5
1	B	484	GLY	6.5
1	A	155	GLY	6.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	485	GLN	6.5
1	C	375	VAL	6.4
1	C	132	SER	6.4
1	C	383	SER	6.3
1	B	289	SER	6.3
1	D	379	GLY	6.3
1	B	164	SER	6.3
1	A	484	GLY	6.3
1	B	379	GLY	6.3
1	A	535	ILE	6.2
1	C	426	VAL	6.2
1	A	486	ARG	6.2
1	D	537	HIS	6.2
1	D	381	GLY	6.2
1	A	45	LEU	6.1
1	C	480	LEU	6.1
1	A	462	PHE	6.1
1	B	269	ALA	6.1
1	B	480	LEU	6.0
1	D	404	GLY	6.0
1	A	384	THR	5.9
1	D	457	ALA	5.9
1	A	250	ILE	5.9
1	D	479	VAL	5.9
1	C	269	ALA	5.9
1	B	498	ASP	5.8
1	A	538	ARG	5.8
1	C	429	PHE	5.8
1	A	378	SER	5.8
1	C	386	ALA	5.8
1	A	358	ALA	5.7
1	A	416	ARG	5.7
1	D	429	PHE	5.6
1	A	379	GLY	5.6
1	B	554	GLY	5.5
1	D	61	ARG	5.5
1	D	511	LEU	5.5
1	D	398	GLY	5.4
1	C	387	SER	5.4
1	D	510	ALA	5.4
1	C	274	SER	5.4
1	D	482	SER	5.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	553	ASP	5.4
1	B	429	PHE	5.4
1	C	481	LEU	5.4
1	B	486	ARG	5.3
1	D	374	LEU	5.3
1	A	350	THR	5.3
1	A	550	VAL	5.3
1	D	420	ALA	5.2
1	C	270	ALA	5.2
1	B	511	LEU	5.2
1	D	486	ARG	5.2
1	D	350	THR	5.1
1	B	286	VAL	5.1
1	B	356	VAL	5.1
1	D	462	PHE	5.1
1	B	481	LEU	5.1
1	B	483	GLY	5.1
1	C	445	TYR	5.0
1	C	482	SER	5.0
1	C	351	TYR	4.9
1	C	479	VAL	4.9
1	B	57	GLY	4.9
1	A	481	LEU	4.9
1	A	511	LEU	4.8
1	B	386	ALA	4.7
1	C	358	ALA	4.7
1	B	482	SER	4.7
1	A	56	PHE	4.7
1	C	511	LEU	4.6
1	A	554	GLY	4.6
1	A	537	HIS	4.6
1	A	55	GLY	4.6
1	A	376	GLY	4.6
1	D	375	VAL	4.6
1	A	532	SER	4.6
1	B	358	ALA	4.5
1	D	359	LEU	4.5
1	B	384	THR	4.5
1	D	384	THR	4.5
1	B	55	GLY	4.4
1	B	380	SER	4.4
1	C	384	THR	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	483	GLY	4.3
1	A	380	SER	4.2
1	A	485	GLN	4.2
1	B	375	VAL	4.1
1	A	479	VAL	4.1
1	C	512	ASP	4.1
1	A	381	GLY	4.1
1	D	540	SER	4.0
1	A	483	GLY	4.0
1	B	537	HIS	3.9
1	D	484	GLY	3.9
1	C	485	GLN	3.9
1	A	482	SER	3.8
1	A	132	SER	3.8
1	A	404	GLY	3.7
1	B	147	VAL	3.7
1	C	379	GLY	3.6
1	C	376	GLY	3.4
1	C	380	SER	3.4
1	D	60	ASP	3.4
1	D	481	LEU	3.4
1	D	358	ALA	3.3
1	B	385	ILE	3.3
1	C	553	ASP	3.3
1	B	378	SER	3.2
1	C	378	SER	3.2
1	B	38	ALA	3.1
1	A	385	ILE	3.0
1	A	354	ARG	2.9
1	D	376	GLY	2.8
1	D	378	SER	2.5
1	B	355	GLU	2.5
1	D	385	ILE	2.5
1	B	376	GLY	2.2
1	C	385	ILE	2.2

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	ANP	D	5003	31/31	1.10	-0.46	219,219,219,219	0
2	ANP	C	5004	31/31	1.11	-0.68	219,219,219,219	0
2	ANP	B	5001	31/31	1.21	-0.69	219,219,219,219	0
2	ANP	A	5002	31/31	1.14	-0.75	219,219,219,219	0

6.5 Other polymers

There are no such residues in this entry.