



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:34 AM GMT

PDB ID : 3PAW
Title : Low resolution X-ray crystal structure of Yeast Rnr1p with dATP bound in the A-site
Authors : Fairman, J.W.; Wijerathna, S.R.; Dealwis, C.G.
Deposited on : 2010-10-19
Resolution : 6.61 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

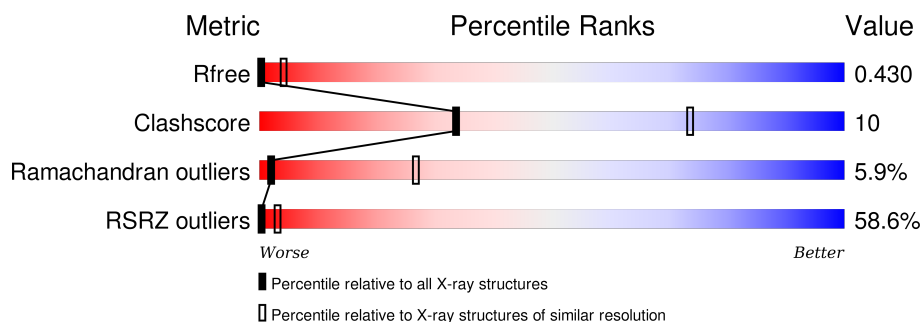
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.61 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1014 (9.50-3.66)
Clashscore	102246	1062 (9.50-3.70)
Ramachandran outliers	100387	1035 (9.50-3.66)
RSRZ outliers	91569	1013 (9.50-3.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	888	
1	B	888	
1	C	888	
1	D	888	

2 Entry composition

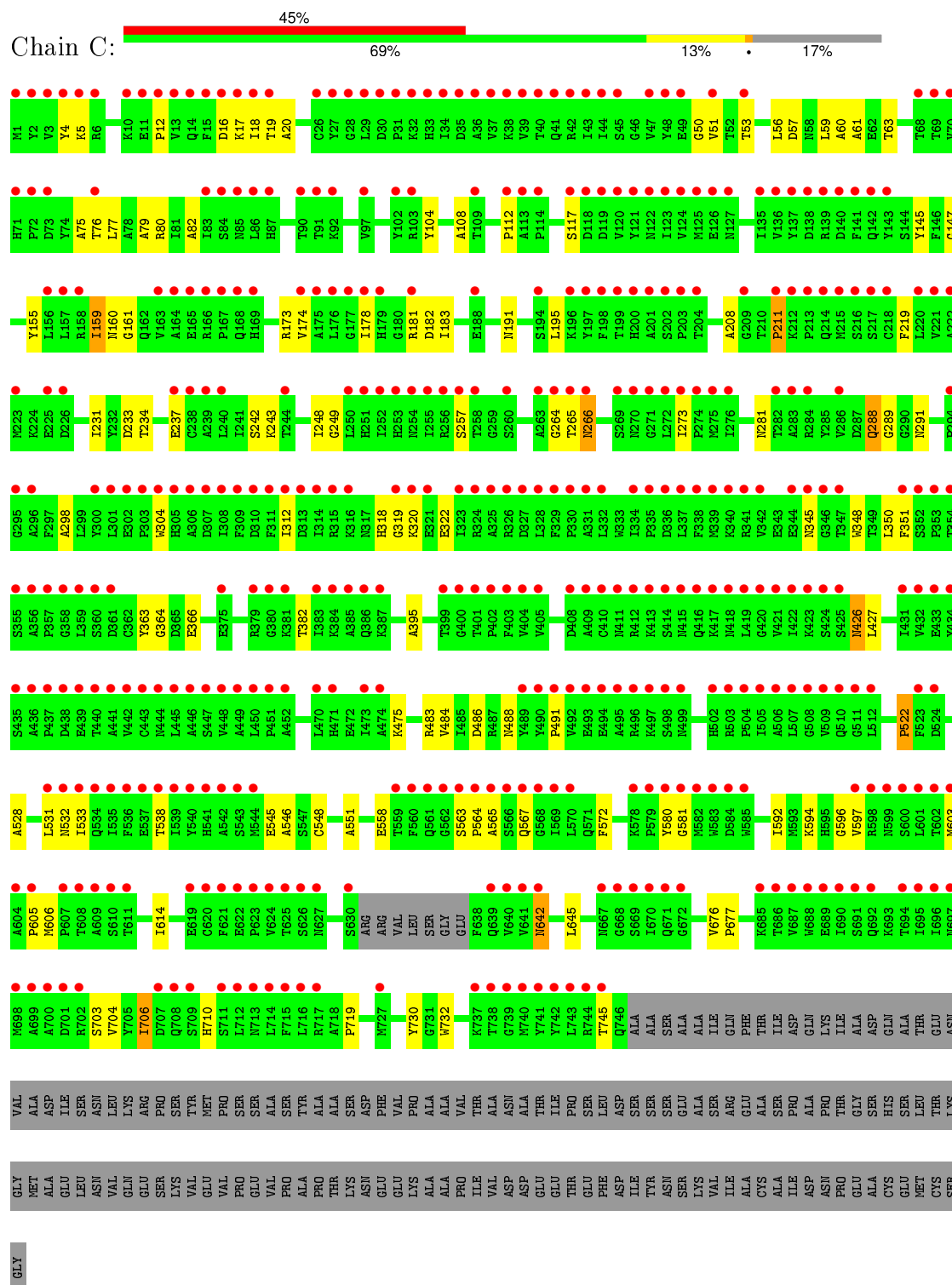
There is only 1 type of molecule in this entry. The entry contains 14596 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Ribonucleoside-diphosphate reductase large chain 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	739	Total	C	N	O	0	0	0
			3649	2171	739	739			
1	B	739	Total	C	N	O	0	0	0
			3649	2171	739	739			
1	C	739	Total	C	N	O	0	0	0
			3649	2171	739	739			
1	D	739	Total	C	N	O	0	0	0
			3649	2171	739	739			

- Molecule 1: Ribonucleoside-diphosphate reductase large chain 1



- Molecule 1: Ribonucleoside-diphosphate reductase large chain 1



VAL	TTR	HT10	R647	M800	C429	P361	A298	E237	H169	D73	M1
GLU	MET	S711	D648	R501	E430	C362	L299	C238	L170	T74	T2
VAL	PRO	L712	L649	H502	V431	T363	T300	A239	V174	A75	V3
PRO	SER	N713	V650	R503	V432	G364	L301	L240	V175	T76	Y4
GLU	SER	N714	D651	P504	E433	D365	E302	I241	L176	L77	R5
VAL	ALA	L715	L652	I505	Y434	E366	E303	S242	L177	A78	R6
SER	SER	L716	G653	I506	S435	F367	R304	K243	G177	A79	D7
TTR	TTR		D654	L507	A436	E368	R305	T244	H178		G8
ALA	ALA	P719	I655	G508	P437	A369	A306	T245	H179		R9
PRO	ALA		D586	V509	D438	L370	D307	G246	G180		R10
TTR	SER			Q510	E439	Y371	L308	G247	R181		E11
LYS	ASP	T725		G511	T440	T372	F309	I248	D182		P12
ASN	ASP	S726		I512	A441	R373	D310	G249	T90		V13
GLU	PHE	M727		A513	V442	T374	F311	L250	T91		Q14
GLU	VAL	H728		D514	C443	E375	L312	H251	K92		F15
LYS	ALA			T515	N444		D313	R252	D100		D16
ALA	ALA	G731		L518	L445	R379	R314	E253			H18
ALA	ALA			L519	A446	K381	R315	N254	Y104		R21
PRO	VAL	L736		P222	A447	T382	K316	I255	L195		L29
ILE	TTR	K737		P523	V448	T383	R317	R256	K196		P31
VAL	ASN	T738		D524	A449	L384	R318	T258	Y197		K32
ASP	ALA	L670		P605	P451	A385	G319	G259	P198		P33
GLU	TTR	G672		L531	A452	Q386	E322	S260	F199		K33
ILE	PRO	L673		N532	F453	K387	R323	Y261	H200		R33
TTR	PRO	L743		I533	I454	L388	R324	I262	A201		I34
GLU	SER	R744		T534	E455	F389	A325	A263	D18		D35
PHE	LEU	T745		I535	S457	Q391	R326	G264	S202		A36
ASP	ASP	Q746		T538	S458	L392	D327	T265	T203		V37
ILE	SER				D459	L393	F329	N266	L205		K38
LYS	SER			A542	T462	E394	R330	G267	F206		V39
ALA	ALA			S543	S463	G400	A331	T268	A208		T40
SER	GLU			M544	T464	T401	L332	S269	G209		Q41
ALA	ALA			E545	Y465	P402	N333	N270	R42		I43
VAL	ILE			A546	N466	F403	I334	G271	T210		I44
ALA	GLU			S547		V404	P335	L272	P211		I44
CYS	ALA			C548	H471	V406	D336	I273	K212		G46
ALA	SER			E549		Y405	L337	P274	P213		G46
ILE	PRO			L550	A474	K407	F338	R275	Q142		V47
ASN	ALA			A551	K475	D408	K339	V278	Y143		Y48
PRO	PRO			P556	A476	A409	R341	N280	Y145		E49
GLU	GLY			Y557	N480	C410	V242	N281	F146		G50
ALA	SER			E558	L481	N411	E343	T282	G147		V51
CYS	HIS			T559	N482	R412	E344	N283	L151		T52
GLU	SER			F560	R483	R413	N345	R284	E152		T53
MET	LEU			Q561	V484	S414	N346	Y285	R153		L56
CYS	TTR			S562	I485	N415	T349	V286	S154		A60
LYS	LYS			S563	Y489	Q416	L350	D287	Y155		A61
GLY	GLY			P564	Y490	G420	F351	Q288	L156		E62
MET	GLY			A565	P491	V421	S352	G289	L157		T63
ALA	ALA			G568	Y492	I422	P353	G290	R158		C64
GLU	LEU			I569	E493	K423	T354	E229	I159		A65
ASN	ASN			L570	E494	S424	S355	N291	G230		Y66
VAL	ASN			Q571	A495	S425	A356	E293	I231		Y66
LEU	VAL			F572	S498	N426	F357	P294	K292		T68
GLN	GLN			D573	N499	L427	G358	G295	Y163		T68
GLU	GLU			N574		C428	L428	L359	A162		T69
SER	SER						L429	L360	E165		T69
PRO	PRO								R166		H71
LYS	LYS								P167		P72

4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	166.51Å 166.51Å 381.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	192.45 – 6.61 36.56 – 6.61	Depositor EDS
% Data completeness (in resolution range)	87.8 (192.45-6.61) 88.3 (36.56-6.61)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 6.63Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.391 , 0.442 0.370 , 0.430	Depositor DCC
R_{free} test set	469 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	225.0	Xtriage
Anisotropy	0.669	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 170.6	EDS
Estimated twinning fraction	0.437 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.20$	Xtriage
Outliers	0 of 9847 reflections	Xtriage
F_o, F_c correlation	0.64	EDS
Total number of atoms	14596	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [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	0.52	0/3647	0.65	0/5075
1	B	0.52	0/3647	0.65	0/5075
1	C	0.53	0/3647	0.66	0/5075
1	D	0.53	0/3647	0.63	0/5075
All	All	0.52	0/14588	0.65	0/20300

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3649	0	1652	61	0
1	B	3649	0	1652	55	0
1	C	3649	0	1652	58	0
1	D	3649	0	1652	44	0
All	All	14596	0	6608	217	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (217) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:GLY:HA3	1:A:614:ILE:HA	1.42	0.99
1:D:147:GLY:HA2	1:D:614:ILE:HA	1.48	0.95
1:C:603:MET:CB	1:C:706:ILE:HA	1.99	0.92
1:A:147:GLY:CA	1:A:614:ILE:HA	2.02	0.90
1:D:147:GLY:CA	1:D:614:ILE:HA	2.07	0.85
1:B:364:GLY:H	1:B:408:ASP:CB	1.94	0.81
1:D:343:GLU:C	1:D:345:ASN:H	1.84	0.79
1:A:513:ALA:HB2	1:A:623:PRO:HA	1.65	0.78
1:D:515:THR:HA	1:D:518:LEU:CB	2.14	0.77
1:C:57:ASP:HA	1:C:60:ALA:HB3	1.69	0.75
1:B:298:ALA:HB3	1:B:427:LEU:HA	1.70	0.74
1:C:147:GLY:CA	1:C:614:ILE:HA	2.18	0.73
1:D:158:ARG:HA	1:D:163:VAL:HA	1.70	0.72
1:B:660:LYS:C	1:B:662:TYR:H	1.92	0.71
1:D:175:ALA:HB1	1:D:186:ALA:HB1	1.73	0.71
1:C:147:GLY:HA3	1:C:614:ILE:O	1.89	0.71
1:C:147:GLY:HA3	1:C:614:ILE:HA	1.74	0.70
1:C:304:TRP:HA	1:C:350:LEU:HA	1.76	0.68
1:D:232:TYR:HA	1:D:235:LEU:CB	2.23	0.68
1:B:298:ALA:CB	1:B:427:LEU:HA	2.24	0.67
1:C:242:SER:O	1:C:288:GLN:HA	1.94	0.67
1:B:191:ASN:O	1:B:195:LEU:N	2.28	0.67
1:A:242:SER:O	1:A:288:GLN:HA	1.95	0.66
1:C:219:PHE:O	1:C:426:ASN:HA	1.96	0.66
1:D:349:THR:HA	1:D:382:THR:HA	1.77	0.66
1:C:75:ALA:C	1:C:77:LEU:H	2.00	0.64
1:D:151:LEU:HA	1:D:155:TYR:CB	2.27	0.64
1:D:474:ALA:HB3	1:D:542:ALA:CB	2.27	0.64
1:A:607:PRO:HA	1:A:620:CYS:CB	2.28	0.64
1:B:287:ASP:HA	1:B:294:PRO:HA	1.81	0.63
1:C:363:TYR:O	1:C:366:GLU:N	2.31	0.62
1:C:191:ASN:O	1:C:195:LEU:N	2.26	0.62
1:D:1:MET:O	1:D:12:PRO:HA	2.00	0.62
1:B:628:MET:HA	1:B:640:VAL:O	2.00	0.61
1:A:27:TYR:C	1:A:29:LEU:H	2.03	0.61
1:B:67:MET:C	1:B:69:THR:H	2.04	0.61
1:C:563:SER:C	1:C:565:ALA:H	2.04	0.61
1:D:3:VAL:N	1:D:11:GLU:O	2.34	0.61
1:C:159:ILE:C	1:C:161:GLY:H	2.04	0.61
1:C:348:TRP:O	1:C:382:THR:HA	2.01	0.60
1:D:304:TRP:O	1:D:350:LEU:HA	2.01	0.60
1:D:474:ALA:HB3	1:D:542:ALA:HB3	1.83	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:ASP:O	1:C:20:ALA:HB2	2.02	0.59
1:A:2:TYR:HA	1:A:11:GLU:O	2.03	0.59
1:C:174:VAL:HA	1:C:208:ALA:HB3	1.85	0.59
1:C:248:ILE:O	1:C:298:ALA:N	2.35	0.59
1:A:217:SER:N	1:A:443:CYS:O	2.35	0.59
1:A:198:PHE:CB	1:A:448:VAL:HA	2.32	0.58
1:A:119:ASP:C	1:A:121:TYR:H	2.07	0.58
1:B:627:ASN:N	1:B:668:GLY:HA3	2.18	0.58
1:C:484:VAL:O	1:C:488:ASN:CB	2.52	0.57
1:C:147:GLY:HA3	1:C:614:ILE:CA	2.35	0.57
1:A:280:ASN:HA	1:A:283:ALA:HB3	1.84	0.57
1:B:471:HIS:HA	1:B:538:THR:O	2.04	0.56
1:B:723:LYS:C	1:B:725:THR:H	2.09	0.56
1:D:343:GLU:C	1:D:345:ASN:N	2.57	0.56
1:C:563:SER:C	1:C:565:ALA:N	2.59	0.56
1:A:273:ILE:C	1:A:275:MET:H	2.09	0.56
1:C:312:ILE:O	1:C:395:ALA:HB1	2.05	0.56
1:B:20:ALA:C	1:B:22:ILE:H	2.08	0.56
1:C:605:PRO:O	1:C:710:HIS:HA	2.06	0.56
1:D:240:LEU:HA	1:D:243:LYS:CB	2.35	0.56
1:D:104:TYR:O	1:D:112:PRO:HA	2.06	0.56
1:A:226:ASP:O	1:A:227:SER:CB	2.55	0.55
1:A:514:ASP:O	1:A:518:LEU:CB	2.55	0.55
1:B:407:LYS:C	1:B:409:ALA:H	2.11	0.54
1:D:563:SER:O	1:D:565:ALA:N	2.37	0.54
1:B:249:GLY:HA3	1:B:426:ASN:C	2.27	0.54
1:A:65:ALA:C	1:A:67:MET:H	2.09	0.54
1:C:104:TYR:O	1:C:112:PRO:HA	2.08	0.53
1:A:298:ALA:HA	1:A:329:PHE:O	2.08	0.53
1:B:251:HIS:CB	1:B:424:SER:CB	2.87	0.53
1:D:612:SER:CB	1:D:619:GLU:HA	2.38	0.53
1:C:548:CYS:HA	1:C:597:VAL:HA	1.90	0.53
1:A:147:GLY:HA2	1:A:614:ILE:HA	1.88	0.53
1:C:57:ASP:O	1:C:61:ALA:N	2.36	0.53
1:B:86:LEU:C	1:B:88:LYS:H	2.12	0.53
1:A:249:GLY:HA2	1:A:298:ALA:O	2.09	0.53
1:B:660:LYS:C	1:B:662:TYR:N	2.62	0.52
1:C:545:GLU:HA	1:C:548:CYS:CB	2.39	0.52
1:D:343:GLU:O	1:D:345:ASN:N	2.42	0.52
1:C:147:GLY:HA3	1:C:614:ILE:C	2.29	0.52
1:D:257:SER:C	1:D:271:GLY:HA2	2.29	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:ALA:HB1	1:A:186:ALA:O	2.10	0.52
1:D:514:ASP:O	1:D:518:LEU:N	2.43	0.52
1:A:523:PHE:H	1:A:683:LEU:HA	1.74	0.52
1:A:508:GLY:HA3	1:A:605:PRO:HA	1.91	0.52
1:D:334:ILE:O	1:D:406:TYR:HA	2.10	0.52
1:B:304:TRP:O	1:B:351:PHE:N	2.42	0.52
1:A:197:TYR:HA	1:A:452:ALA:CB	2.40	0.52
1:D:513:ALA:HB2	1:D:623:PRO:HA	1.92	0.52
1:C:572:PHE:N	1:C:704:VAL:O	2.43	0.51
1:A:224:LYS:O	1:A:225:GLU:CB	2.58	0.51
1:C:249:GLY:HA2	1:C:298:ALA:O	2.10	0.51
1:C:243:LYS:HA	1:C:289:GLY:H	1.76	0.51
1:C:61:ALA:HB1	1:C:82:ALA:HB2	1.93	0.51
1:D:226:ASP:O	1:D:227:SER:CB	2.59	0.51
1:D:234:THR:HA	1:D:237:GLU:CB	2.41	0.50
1:C:17:LYS:C	1:C:19:THR:H	2.14	0.50
1:A:196:LYS:O	1:A:449:ALA:HB3	2.12	0.50
1:D:147:GLY:HA3	1:D:614:ILE:HA	1.91	0.50
1:B:363:TYR:O	1:B:366:GLU:N	2.40	0.50
1:B:725:THR:C	1:B:727:MET:H	2.16	0.49
1:C:298:ALA:HB3	1:C:427:LEU:HA	1.95	0.49
1:A:299:LEU:O	1:A:331:ALA:N	2.41	0.49
1:C:75:ALA:C	1:C:77:LEU:N	2.64	0.49
1:A:27:TYR:O	1:A:29:LEU:N	2.40	0.49
1:B:75:ALA:C	1:B:77:LEU:H	2.15	0.49
1:A:16:ASP:O	1:A:20:ALA:HB2	2.12	0.49
1:A:538:THR:O	1:A:542:ALA:N	2.46	0.49
1:A:312:ILE:O	1:A:395:ALA:HB1	2.12	0.49
1:C:117:SER:HA	1:C:211:PRO:HA	1.95	0.48
1:D:474:ALA:HB3	1:D:542:ALA:HB1	1.95	0.48
1:C:77:LEU:HA	1:C:80:ARG:CB	2.44	0.48
1:C:281:ASN:CB	1:D:278:VAL:HA	2.43	0.48
1:D:301:LEU:O	1:D:332:LEU:HA	2.13	0.48
1:D:61:ALA:CB	1:D:82:ALA:HB2	2.42	0.48
1:A:375:GLU:C	1:A:377:GLU:H	2.16	0.47
1:B:505:ILE:N	1:B:601:LEU:O	2.41	0.47
1:B:20:ALA:C	1:B:22:ILE:N	2.66	0.47
1:C:173:ARG:O	1:C:208:ALA:O	2.31	0.47
1:D:661:GLN:C	1:D:663:LEU:H	2.18	0.47
1:D:53:THR:HA	1:D:56:LEU:CB	2.45	0.47
1:A:52:THR:O	1:A:56:LEU:N	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:THR:HA	1:C:237:GLU:CB	2.45	0.47
1:C:53:THR:HA	1:C:56:LEU:CB	2.44	0.47
1:C:265:THR:O	1:C:266:ASN:CB	2.62	0.47
1:C:592:ILE:C	1:C:594:LYS:N	2.67	0.47
1:A:300:TYR:HA	1:A:331:ALA:O	2.14	0.47
1:D:505:ILE:O	1:D:601:LEU:O	2.33	0.47
1:B:257:SER:CB	1:B:306:ALA:HB3	2.45	0.47
1:B:301:LEU:O	1:B:333:TRP:N	2.47	0.46
1:A:279:PHE:O	1:A:283:ALA:N	2.46	0.46
1:A:197:TYR:HA	1:A:452:ALA:HB1	1.97	0.46
1:C:522:PRO:O	1:C:528:ALA:HB1	2.15	0.46
1:B:39:VAL:O	1:B:42:ARG:N	2.49	0.46
1:A:359:LEU:C	1:A:361:ASP:H	2.18	0.46
1:A:64:CYS:CB	1:A:78:ALA:HB2	2.46	0.46
1:B:231:ILE:C	1:B:233:ASP:H	2.17	0.46
1:A:349:THR:HA	1:A:382:THR:HA	1.98	0.46
1:A:339:MET:C	1:A:341:ARG:H	2.19	0.46
1:B:287:ASP:HA	1:B:294:PRO:CA	2.45	0.46
1:D:471:HIS:HA	1:D:542:ALA:HB2	1.98	0.45
1:A:474:ALA:HB3	1:A:542:ALA:HB1	1.98	0.45
1:D:373:ARG:C	1:D:375:GLU:H	2.19	0.45
1:B:213:PRO:O	1:B:489:TYR:N	2.49	0.45
1:B:404:VAL:O	1:B:739:GLY:N	2.49	0.45
1:B:721:MET:C	1:B:723:LYS:H	2.18	0.45
1:B:572:PHE:N	1:B:704:VAL:O	2.49	0.45
1:B:445:LEU:O	1:B:446:ALA:HB2	2.17	0.45
1:B:65:ALA:C	1:B:67:MET:H	2.20	0.45
1:C:181:ARG:O	1:C:183:ILE:N	2.49	0.45
1:B:694:THR:C	1:B:696:ILE:H	2.20	0.45
1:B:67:MET:C	1:B:69:THR:N	2.69	0.45
1:A:65:ALA:O	1:A:67:MET:N	2.50	0.45
1:C:592:ILE:HA	1:C:596:GLY:H	1.82	0.45
1:A:60:ALA:C	1:A:62:GLU:H	2.20	0.45
1:C:174:VAL:HA	1:C:208:ALA:CB	2.47	0.44
1:A:104:TYR:O	1:A:113:ALA:N	2.34	0.44
1:A:513:ALA:HB3	1:A:618:ASN:CB	2.47	0.44
1:A:60:ALA:C	1:A:62:GLU:N	2.70	0.44
1:D:249:GLY:HA2	1:D:298:ALA:H	1.81	0.44
1:C:231:ILE:C	1:C:233:ASP:H	2.21	0.44
1:A:59:LEU:O	1:A:63:THR:N	2.50	0.44
1:B:212:LYS:O	1:B:214:GLN:N	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:531:LEU:C	1:C:533:ILE:H	2.21	0.44
1:D:457:SER:O	1:D:459:ASP:N	2.48	0.44
1:A:425:SER:HA	1:A:431:ILE:O	2.17	0.44
1:B:730:TYR:C	1:B:732:TRP:H	2.21	0.44
1:B:335:PRO:C	1:B:337:LEU:H	2.20	0.44
1:A:486:ASP:O	1:A:488:ASN:N	2.51	0.44
1:A:277:ARG:HA	1:A:280:ASN:CB	2.48	0.43
1:D:538:THR:O	1:D:542:ALA:N	2.52	0.43
1:A:287:ASP:O	1:A:290:GLY:N	2.52	0.43
1:B:62:GLU:O	1:B:65:ALA:HB3	2.18	0.43
1:C:159:ILE:C	1:C:161:GLY:N	2.72	0.43
1:A:299:LEU:N	1:A:329:PHE:O	2.51	0.43
1:B:392:ILE:C	1:B:394:GLU:H	2.22	0.43
1:A:506:ALA:CB	1:A:604:ALA:HB3	2.49	0.43
1:A:493:GLU:O	1:A:497:LYS:N	2.49	0.43
1:B:531:LEU:C	1:B:533:ILE:H	2.22	0.43
1:C:563:SER:O	1:C:565:ALA:N	2.52	0.43
1:C:59:LEU:O	1:C:63:THR:N	2.51	0.43
1:A:486:ASP:C	1:A:488:ASN:H	2.23	0.42
1:C:703:SER:HA	1:C:706:ILE:CB	2.49	0.42
1:A:22:ILE:O	1:A:26:CYS:N	2.53	0.42
1:C:79:ALA:HA	1:C:82:ALA:HB3	2.01	0.42
1:D:406:TYR:CB	1:D:409:ALA:HB3	2.49	0.42
1:C:475:LYS:HA	1:C:546:ALA:HB2	2.01	0.42
1:B:565:ALA:HA	1:B:569:ILE:O	2.19	0.42
1:C:730:TYR:C	1:C:732:TRP:H	2.23	0.42
1:A:65:ALA:C	1:A:67:MET:N	2.73	0.42
1:C:483:ARG:HA	1:C:486:ASP:CB	2.49	0.42
1:B:147:GLY:HA2	1:B:614:ILE:HA	2.01	0.42
1:B:627:ASN:O	1:B:641:VAL:HA	2.20	0.41
1:A:243:LYS:O	1:A:289:GLY:N	2.52	0.41
1:B:283:ALA:HB1	1:B:295:GLY:O	2.19	0.41
1:B:303:PRO:C	1:B:305:HIS:H	2.24	0.41
1:C:642:ASN:CB	1:C:645:LEU:CB	2.98	0.41
1:D:231:ILE:O	1:D:235:LEU:N	2.54	0.41
1:C:551:ALA:HB2	1:C:597:VAL:C	2.40	0.41
1:D:475:LYS:HA	1:D:546:ALA:HB2	2.02	0.41
1:A:27:TYR:C	1:A:29:LEU:N	2.70	0.41
1:A:287:ASP:O	1:A:289:GLY:N	2.53	0.41
1:D:248:ILE:O	1:D:297:PHE:HA	2.20	0.41
1:B:75:ALA:C	1:B:77:LEU:N	2.74	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:SER:HA	1:B:394:GLU:CB	2.50	0.41
1:A:148:PHE:C	1:A:150:THR:N	2.75	0.41
1:A:76:THR:HA	1:A:79:ALA:HB3	2.02	0.40
1:A:5:LYS:C	1:A:7:ASP:H	2.24	0.40
1:B:371:TYR:C	1:B:373:ARG:H	2.25	0.40
1:B:280:ASN:C	1:B:282:THR:H	2.25	0.40
1:B:204:THR:O	1:B:208:ALA:HB2	2.21	0.40
1:B:405:VAL:HA	1:B:738:THR:HA	2.03	0.40
1:D:304:TRP:O	1:D:351:PHE:N	2.55	0.40
1:B:680:LEU:HA	1:B:683:LEU:CB	2.51	0.40
1:B:83:ILE:C	1:B:85:ASN:H	2.25	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	735/888 (83%)	533 (72%)	157 (21%)	45 (6%)	2	26
1	B	735/888 (83%)	518 (70%)	180 (24%)	37 (5%)	3	31
1	C	735/888 (83%)	536 (73%)	154 (21%)	45 (6%)	2	26
1	D	735/888 (83%)	542 (74%)	148 (20%)	45 (6%)	2	26
All	All	2940/3552 (83%)	2129 (72%)	639 (22%)	172 (6%)	2	27

All (172) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	225	GLU
1	A	227	SER
1	A	288	GLN
1	A	461	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	486	ASP
1	A	677	PRO
1	B	501	ARG
1	B	719	PRO
1	C	5	LYS
1	C	145	TYR
1	C	291	ASN
1	C	318	HIS
1	C	320	LYS
1	D	5	LYS
1	D	196	LYS
1	D	227	SER
1	D	291	ASN
1	D	667	ASN
1	D	677	PRO
1	A	120	VAL
1	A	290	GLY
1	A	487	ARG
1	A	558	GLU
1	A	613	GLN
1	A	623	PRO
1	A	674	PRO
1	B	159	ILE
1	B	364	GLY
1	B	452	ALA
1	C	108	ALA
1	C	159	ILE
1	C	182	ASP
1	C	288	GLN
1	C	319	GLY
1	C	364	GLY
1	C	491	PRO
1	C	706	ILE
1	D	159	ILE
1	D	206	PHE
1	D	288	GLN
1	D	318	HIS
1	D	319	GLY
1	D	343	GLU
1	D	344	GLU
1	D	522	PRO
1	D	719	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	6	ARG
1	A	8	GLY
1	A	66	TYR
1	A	201	ALA
1	A	259	GLY
1	A	353	PRO
1	A	501	ARG
1	A	679	GLU
1	A	708	GLN
1	A	741	TYR
1	B	50	GLY
1	B	87	HIS
1	B	109	THR
1	B	175	ALA
1	B	264	GLY
1	B	345	ASN
1	B	437	PRO
1	B	626	SER
1	B	740	MET
1	B	745	THR
1	C	4	TYR
1	C	12	PRO
1	C	160	ASN
1	C	266	ASN
1	C	273	ILE
1	C	322	GLU
1	C	426	ASN
1	C	522	PRO
1	C	532	ASN
1	C	581	GLY
1	C	606	MET
1	D	145	TYR
1	D	257	SER
1	D	266	ASN
1	D	345	ASN
1	D	462	THR
1	D	609	ALA
1	D	686	THR
1	A	153	ARG
1	A	159	ILE
1	A	304	TRP
1	A	318	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	492	VAL
1	A	608	THR
1	A	657	GLU
1	B	8	GLY
1	B	12	PRO
1	B	191	ASN
1	B	266	ASN
1	B	304	TRP
1	B	458	GLU
1	B	580	TYR
1	B	656	ASP
1	B	737	LYS
1	C	76	THR
1	C	155	TYR
1	C	211	PRO
1	C	345	ASN
1	C	558	GLU
1	C	564	PRO
1	C	567	GLN
1	C	719	PRO
1	C	745	THR
1	D	50	GLY
1	D	119	ASP
1	D	259	GLY
1	D	264	GLY
1	D	458	GLU
1	D	493	GLU
1	D	582	MET
1	D	586	ASP
1	D	662	TYR
1	D	741	TYR
1	A	110	GLY
1	A	160	ASN
1	A	345	ASN
1	A	460	GLY
1	A	571	GLN
1	B	93	GLN
1	B	210	THR
1	B	273	ILE
1	B	387	LYS
1	B	459	ASP
1	B	558	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	617	TYR
1	B	620	CYS
1	B	661	GLN
1	C	18	ILE
1	C	257	SER
1	C	264	GLY
1	C	351	PHE
1	C	538	THR
1	C	580	TYR
1	C	642	ASN
1	D	292	LYS
1	D	353	PRO
1	D	579	PRO
1	D	737	LYS
1	A	266	ASN
1	A	417	LYS
1	A	511	GLY
1	C	51	VAL
1	D	114	PRO
1	D	153	ARG
1	D	374	TYR
1	D	684	TYR
1	A	28	GLY
1	A	274	PRO
1	C	50	GLY
1	A	564	PRO
1	B	31	PRO
1	B	180	GLY
1	B	213	PRO
1	C	676	VAL
1	D	203	PRO
1	D	511	GLY
1	A	30	ASP
1	A	241	ILE
1	A	276	ILE
1	B	454	ILE
1	C	677	PRO
1	D	491	PRO
1	D	623	PRO
1	D	690	ILE
1	A	163	VAL
1	C	178	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 molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	739/888 (83%)	3.34	458 (61%) 0 3	39, 81, 170, 183	0
1	B	739/888 (83%)	2.85	388 (52%) 0 4	52, 74, 175, 188	0
1	C	739/888 (83%)	3.11	403 (54%) 0 3	51, 73, 173, 194	0
1	D	739/888 (83%)	3.55	483 (65%) 0 3	58, 80, 175, 186	0
All	All	2956/3552 (83%)	3.21	1732 (58%) 0 3	39, 78, 173, 194	0

All (1732) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	711	SER	18.8
1	C	433	GLU	18.8
1	B	415	ASN	18.6
1	B	414	SER	17.5
1	D	218	CYS	17.2
1	B	510	GLN	17.1
1	C	415	ASN	16.8
1	D	596	GLY	16.5
1	B	220	LEU	16.0
1	A	441	ALA	15.6
1	D	686	THR	15.4
1	D	219	PHE	15.3
1	D	217	SER	15.2
1	A	605	PRO	15.2
1	A	14	GLN	15.0
1	B	416	GLN	15.0
1	C	215	MET	14.9
1	B	433	GLU	14.8
1	A	557	TYR	14.7
1	C	216	SER	14.6
1	C	686	THR	14.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	442	VAL	14.2
1	C	624	VAL	14.0
1	D	216	SER	13.8
1	D	443	CYS	13.8
1	D	738	THR	13.7
1	A	251	HIS	13.7
1	C	441	ALA	13.5
1	D	605	PRO	13.5
1	D	442	VAL	13.4
1	C	435	SER	13.2
1	A	558	GLU	13.1
1	C	504	PRO	13.0
1	C	508	GLY	13.0
1	B	442	VAL	12.9
1	B	36	ALA	12.9
1	D	220	LEU	12.8
1	C	414	SER	12.7
1	B	509	VAL	12.6
1	D	256	ARG	12.6
1	C	443	CYS	12.6
1	D	710	HIS	12.5
1	A	254	ASN	12.3
1	C	537	GLU	12.3
1	D	685	LYS	12.2
1	D	623	PRO	12.1
1	D	433	GLU	12.1
1	B	219	PHE	12.0
1	B	254	ASN	12.0
1	C	416	GLN	12.0
1	B	14	GLN	11.8
1	A	692	GLN	11.7
1	D	689	GLU	11.7
1	D	286	VAL	11.7
1	A	715	PHE	11.7
1	D	255	ILE	11.7
1	B	136	VAL	11.6
1	B	379	ARG	11.6
1	A	623	PRO	11.6
1	C	625	THR	11.5
1	D	712	LEU	11.5
1	C	220	LEU	11.4
1	C	444	ASN	11.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	385	ALA	11.3
1	C	257	SER	11.2
1	D	284	ARG	11.2
1	D	283	ALA	11.1
1	A	221	VAL	11.0
1	D	441	ALA	11.0
1	D	444	ASN	11.0
1	A	711	SER	11.0
1	A	442	VAL	10.9
1	A	559	THR	10.9
1	C	341	ARG	10.9
1	A	15	PHE	10.9
1	A	250	LEU	10.9
1	D	687	VAL	10.8
1	B	413	LYS	10.8
1	A	220	LEU	10.8
1	C	509	VAL	10.8
1	A	325	ALA	10.7
1	C	599	ASN	10.7
1	C	380	GLY	10.7
1	D	688	TRP	10.6
1	C	440	THR	10.6
1	D	606	MET	10.6
1	C	417	LYS	10.6
1	C	506	ALA	10.6
1	C	434	TYR	10.6
1	C	432	VAL	10.5
1	B	29	LEU	10.5
1	C	214	GLN	10.5
1	D	246	GLY	10.5
1	B	620	CYS	10.5
1	D	690	ILE	10.4
1	C	623	PRO	10.4
1	A	415	ASN	10.4
1	B	432	VAL	10.3
1	A	435	SER	10.3
1	D	739	GLY	10.3
1	B	218	CYS	10.2
1	D	709	SER	10.2
1	B	425	SER	10.2
1	D	90	THR	10.2
1	D	713	ASN	10.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	254	ASN	10.1
1	D	285	TYR	10.1
1	B	713	ASN	10.1
1	B	256	ARG	10.1
1	A	681	LYS	10.1
1	A	710	HIS	10.0
1	B	380	GLY	10.0
1	D	282	THR	10.0
1	D	215	MET	10.0
1	B	443	CYS	10.0
1	B	255	ILE	10.0
1	C	510	GLN	10.0
1	D	547	SER	10.0
1	B	253	HIS	10.0
1	D	694	THR	9.9
1	B	715	PHE	9.9
1	C	505	ILE	9.9
1	C	687	VAL	9.9
1	B	417	LYS	9.9
1	A	738	THR	9.8
1	A	713	ASN	9.8
1	A	302	GLU	9.7
1	D	221	VAL	9.7
1	B	302	GLU	9.6
1	D	165	GLU	9.6
1	C	712	LEU	9.6
1	B	15	PHE	9.6
1	A	712	LEU	9.6
1	D	295	GLY	9.6
1	D	504	PRO	9.5
1	B	623	PRO	9.5
1	B	441	ALA	9.5
1	C	16	ASP	9.5
1	C	494	GLU	9.4
1	C	602	THR	9.4
1	B	622	GLU	9.4
1	C	256	ARG	9.4
1	A	1	MET	9.4
1	D	253	HIS	9.4
1	D	352	SER	9.4
1	D	214	GLN	9.3
1	C	421	VAL	9.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	580	TYR	9.3
1	D	432	VAL	9.3
1	A	606	MET	9.3
1	A	255	ILE	9.2
1	B	424	SER	9.1
1	C	306	ALA	9.1
1	C	422	ILE	9.1
1	D	166	ARG	9.1
1	A	600	SER	9.1
1	B	135	ILE	9.0
1	B	310	ASP	9.0
1	C	253	HIS	9.0
1	A	434	TYR	9.0
1	D	91	THR	8.9
1	A	326	ARG	8.9
1	D	624	VAL	8.9
1	D	289	GLY	8.9
1	C	254	ASN	8.9
1	D	741	TYR	8.8
1	A	599	ASN	8.8
1	B	709	SER	8.8
1	D	198	PHE	8.8
1	C	412	ARG	8.8
1	B	1	MET	8.8
1	D	196	LYS	8.8
1	A	353	PRO	8.8
1	A	714	LEU	8.7
1	C	600	SER	8.7
1	C	532	ASN	8.7
1	C	533	ILE	8.7
1	D	625	THR	8.7
1	A	249	GLY	8.7
1	A	3	VAL	8.7
1	D	421	VAL	8.7
1	C	2	TYR	8.7
1	A	416	GLN	8.7
1	B	16	ASP	8.6
1	A	622	GLU	8.6
1	B	418	ASN	8.6
1	A	739	GLY	8.6
1	C	445	LEU	8.6
1	D	430	GLU	8.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	740	MET	8.6
1	B	708	GLN	8.5
1	D	226	ASP	8.5
1	B	37	VAL	8.5
1	C	30	ASP	8.5
1	A	93	GLN	8.4
1	D	202	SER	8.4
1	A	504	PRO	8.4
1	A	261	TYR	8.4
1	C	29	LEU	8.4
1	A	440	THR	8.4
1	A	327	ASP	8.4
1	C	534	GLN	8.4
1	D	422	ILE	8.3
1	D	569	ILE	8.3
1	D	197	TYR	8.3
1	C	384	LYS	8.3
1	C	4	TYR	8.3
1	B	247	GLY	8.3
1	B	742	TYR	8.3
1	C	423	LYS	8.3
1	B	143	TYR	8.3
1	A	680	LEU	8.2
1	C	601	LEU	8.2
1	A	691	SER	8.2
1	A	260	SER	8.2
1	A	543	SER	8.2
1	B	532	ASN	8.2
1	D	428	CYS	8.2
1	D	247	GLY	8.1
1	D	415	ASN	8.1
1	C	446	ALA	8.1
1	A	556	PRO	8.1
1	B	707	ASP	8.1
1	C	164	ALA	8.1
1	D	302	GLU	8.0
1	D	509	VAL	8.0
1	B	712	LEU	8.0
1	A	72	PRO	8.0
1	A	509	VAL	8.0
1	D	597	VAL	8.0
1	B	710	HIS	8.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	622	GLU	8.0
1	B	309	PHE	7.9
1	A	682	ASP	7.9
1	C	579	PRO	7.9
1	A	737	LYS	7.9
1	C	15	PHE	7.9
1	C	507	LEU	7.9
1	A	73	ASP	7.9
1	A	4	TYR	7.8
1	B	522	PRO	7.8
1	C	536	PHE	7.8
1	C	302	GLU	7.7
1	C	538	THR	7.7
1	D	182	ASP	7.7
1	A	642	ASN	7.7
1	A	194	SER	7.7
1	A	508	GLY	7.7
1	C	411	ASN	7.6
1	A	13	VAL	7.6
1	A	215	MET	7.6
1	B	252	ILE	7.6
1	D	380	GLY	7.6
1	D	503	ARG	7.6
1	B	619	GLU	7.6
1	D	431	ILE	7.5
1	D	510	GLN	7.5
1	B	435	SER	7.5
1	D	463	SER	7.5
1	A	253	HIS	7.5
1	C	270	ASN	7.5
1	D	598	ARG	7.5
1	B	208	ALA	7.5
1	A	424	SER	7.5
1	D	50	GLY	7.5
1	D	451	PRO	7.5
1	B	618	ASN	7.5
1	C	688	TRP	7.5
1	A	716	LEU	7.5
1	A	265	THR	7.4
1	A	142	GLN	7.4
1	D	265	THR	7.4
1	C	740	MET	7.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	691	SER	7.4
1	B	508	GLY	7.4
1	C	535	ILE	7.4
1	B	599	ASN	7.4
1	D	414	SER	7.4
1	A	675	ASN	7.4
1	A	647	ARG	7.3
1	A	16	ASP	7.3
1	C	3	VAL	7.3
1	C	11	GLU	7.3
1	D	684	TYR	7.3
1	A	444	ASN	7.3
1	C	1	MET	7.3
1	A	604	ALA	7.2
1	D	303	PRO	7.2
1	D	353	PRO	7.2
1	B	600	SER	7.2
1	A	743	LEU	7.2
1	B	534	GLN	7.2
1	D	695	ILE	7.2
1	B	50	GLY	7.2
1	D	354	THR	7.2
1	D	227	SER	7.2
1	C	715	PHE	7.2
1	A	252	ILE	7.2
1	A	709	SER	7.1
1	D	648	ASP	7.1
1	D	296	ALA	7.1
1	D	681	LYS	7.1
1	A	443	CYS	7.1
1	D	548	CYS	7.1
1	B	447	SER	7.1
1	D	423	LYS	7.1
1	C	271	GLY	7.0
1	B	431	ILE	7.0
1	C	424	SER	7.0
1	D	705	TYR	7.0
1	B	30	ASP	7.0
1	C	540	TYR	7.0
1	A	30	ASP	7.0
1	A	668	GLY	6.9
1	D	599	ASN	6.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	49	GLU	6.9
1	D	715	PHE	6.9
1	D	327	ASP	6.9
1	B	378	GLY	6.9
1	D	167	PRO	6.9
1	C	352	SER	6.9
1	D	682	ASP	6.9
1	C	418	ASN	6.9
1	C	413	LYS	6.9
1	B	512	LEU	6.9
1	A	580	TYR	6.8
1	B	51	VAL	6.8
1	C	491	PRO	6.8
1	A	143	TYR	6.8
1	D	524	ASP	6.8
1	A	222	ALA	6.7
1	D	491	PRO	6.7
1	A	208	ALA	6.7
1	A	601	LEU	6.7
1	D	490	TYR	6.7
1	A	207	ASN	6.7
1	B	714	LEU	6.7
1	D	137	TYR	6.7
1	C	691	SER	6.7
1	A	683	LEU	6.7
1	C	140	ASP	6.7
1	C	447	SER	6.7
1	A	92	LYS	6.7
1	B	511	GLY	6.6
1	B	249	GLY	6.6
1	B	248	ILE	6.6
1	A	204	THR	6.6
1	D	570	LEU	6.6
1	A	728	HIS	6.6
1	C	578	LYS	6.6
1	D	140	ASP	6.5
1	C	564	PRO	6.5
1	B	175	ALA	6.5
1	C	252	ILE	6.5
1	D	693	LYS	6.5
1	A	643	PRO	6.5
1	C	303	PRO	6.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	426	ASN	6.5
1	A	607	PRO	6.5
1	A	90	THR	6.5
1	D	626	SER	6.5
1	B	250	LEU	6.5
1	A	263	ALA	6.5
1	D	288	GLN	6.4
1	A	12	PRO	6.4
1	D	564	PRO	6.4
1	C	713	ASN	6.4
1	D	692	GLN	6.4
1	D	708	GLN	6.4
1	D	413	LYS	6.4
1	C	741	TYR	6.4
1	D	600	SER	6.4
1	D	508	GLY	6.4
1	D	212	LYS	6.4
1	D	670	ILE	6.4
1	C	581	GLY	6.4
1	B	466	ASN	6.4
1	D	251	HIS	6.4
1	B	535	ILE	6.4
1	D	34	ILE	6.4
1	B	738	THR	6.4
1	A	466	ASN	6.4
1	B	165	GLU	6.4
1	C	565	ALA	6.4
1	C	539	ILE	6.4
1	D	264	GLY	6.3
1	A	684	TYR	6.3
1	A	303	PRO	6.3
1	C	218	CYS	6.3
1	A	264	GLY	6.3
1	A	296	ALA	6.3
1	C	327	ASP	6.3
1	A	300	TYR	6.3
1	A	730	TYR	6.3
1	C	14	GLN	6.3
1	D	30	ASP	6.3
1	A	425	SER	6.3
1	C	420	GLY	6.3
1	D	203	PRO	6.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	311	PHE	6.3
1	C	690	ILE	6.3
1	A	532	ASN	6.3
1	C	668	GLY	6.3
1	D	266	ASN	6.3
1	A	315	ARG	6.3
1	B	624	VAL	6.3
1	C	137	TYR	6.3
1	A	717	ARG	6.3
1	A	127	ASN	6.3
1	D	429	CYS	6.3
1	D	164	ALA	6.2
1	B	603	MET	6.2
1	D	389	TRP	6.2
1	A	523	PHE	6.2
1	C	608	THR	6.2
1	D	201	ALA	6.2
1	C	340	LYS	6.2
1	C	324	ARG	6.2
1	C	12	PRO	6.2
1	D	649	LEU	6.2
1	A	408	ASP	6.2
1	C	436	ALA	6.2
1	D	139	ARG	6.1
1	C	221	VAL	6.1
1	B	246	GLY	6.1
1	D	707	ASP	6.1
1	D	607	PRO	6.1
1	D	571	GLN	6.1
1	B	92	LYS	6.1
1	C	91	THR	6.1
1	A	140	ASP	6.1
1	A	286	VAL	6.1
1	A	546	ALA	6.1
1	D	355	SER	6.1
1	A	406	TYR	6.1
1	B	611	THR	6.1
1	A	579	PRO	6.1
1	A	727	MET	6.1
1	C	495	ALA	6.1
1	A	266	ASN	6.0
1	A	295	GLY	6.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	360	SER	6.0
1	A	2	TYR	6.0
1	A	262	ILE	6.0
1	D	179	HIS	6.0
1	C	251	HIS	6.0
1	C	5	LYS	6.0
1	A	423	LYS	6.0
1	C	177	GLY	6.0
1	C	307	ASP	6.0
1	D	532	ASN	6.0
1	C	449	ALA	6.0
1	B	450	LEU	6.0
1	C	739	GLY	6.0
1	B	533	ILE	6.0
1	C	255	ILE	6.0
1	C	165	GLU	5.9
1	B	207	ASN	5.9
1	D	601	LEU	5.9
1	D	213	PRO	5.9
1	A	352	SER	5.9
1	A	620	CYS	5.9
1	A	676	VAL	5.9
1	B	579	PRO	5.9
1	B	669	SER	5.9
1	A	421	VAL	5.9
1	D	511	GLY	5.9
1	A	524	ASP	5.9
1	D	200	HIS	5.9
1	D	683	LEU	5.9
1	B	536	PHE	5.9
1	D	678	GLN	5.9
1	C	136	VAL	5.9
1	B	2	TYR	5.9
1	A	446	ALA	5.8
1	C	274	PRO	5.8
1	A	542	ALA	5.8
1	A	679	GLU	5.8
1	C	410	CYS	5.8
1	C	670	ILE	5.8
1	A	174	VAL	5.8
1	A	256	ARG	5.8
1	C	339	MET	5.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	671	GLN	5.8
1	A	168	GLN	5.8
1	D	204	THR	5.8
1	A	533	ILE	5.8
1	B	711	SER	5.8
1	C	493	GLU	5.8
1	B	385	ALA	5.8
1	C	716	LEU	5.8
1	C	338	PHE	5.7
1	A	694	THR	5.7
1	A	641	VAL	5.7
1	A	428	CYS	5.7
1	D	207	ASN	5.7
1	C	503	ARG	5.7
1	A	731	GLY	5.7
1	A	646	LEU	5.7
1	B	703	SER	5.7
1	A	304	TRP	5.7
1	C	142	GLN	5.7
1	D	604	ALA	5.7
1	D	357	PRO	5.7
1	B	449	ALA	5.7
1	D	745	THR	5.7
1	C	336	ASP	5.7
1	A	534	GLN	5.7
1	B	604	ALA	5.7
1	A	448	VAL	5.7
1	C	305	HIS	5.7
1	A	173	ARG	5.6
1	A	703	SER	5.6
1	B	295	GLY	5.6
1	C	641	VAL	5.6
1	D	669	SER	5.6
1	B	251	HIS	5.6
1	C	622	GLU	5.6
1	B	446	ALA	5.6
1	C	212	LYS	5.6
1	D	136	VAL	5.6
1	D	484	VAL	5.6
1	B	140	ASP	5.6
1	B	265	THR	5.6
1	B	621	PHE	5.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	595	HIS	5.6
1	C	492	VAL	5.6
1	D	679	GLU	5.6
1	B	381	LYS	5.6
1	C	258	THR	5.6
1	C	33	HIS	5.6
1	D	737	LYS	5.6
1	A	85	ASN	5.6
1	B	38	LYS	5.6
1	D	199	THR	5.6
1	D	742	TYR	5.6
1	A	433	GLU	5.6
1	D	245	ALA	5.6
1	A	171	ILE	5.6
1	B	200	HIS	5.6
1	B	35	ASP	5.6
1	C	563	SER	5.5
1	A	674	PRO	5.5
1	B	199	THR	5.5
1	A	400	GLY	5.5
1	C	610	SER	5.5
1	B	49	GLU	5.5
1	C	351	PHE	5.5
1	D	714	LEU	5.5
1	A	420	GLY	5.5
1	C	448	VAL	5.5
1	C	328	LEU	5.5
1	C	738	THR	5.5
1	A	71	HIS	5.5
1	A	219	PHE	5.5
1	A	744	ARG	5.5
1	A	445	LEU	5.5
1	D	356	ALA	5.5
1	C	439	GLU	5.4
1	D	195	LEU	5.4
1	C	272	LEU	5.4
1	A	513	ALA	5.4
1	B	412	ARG	5.4
1	C	296	ALA	5.4
1	A	544	MET	5.4
1	C	404	VAL	5.4
1	B	537	GLU	5.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	354	THR	5.4
1	A	602	THR	5.4
1	B	273	ILE	5.4
1	B	538	THR	5.4
1	B	13	VAL	5.4
1	C	273	ILE	5.4
1	A	598	ARG	5.4
1	A	285	TYR	5.4
1	B	222	ALA	5.4
1	C	708	GLN	5.4
1	B	670	ILE	5.4
1	B	434	TYR	5.4
1	A	439	GLU	5.4
1	C	402	PRO	5.4
1	C	345	ASN	5.4
1	A	512	LEU	5.3
1	C	143	TYR	5.3
1	C	744	ARG	5.3
1	B	444	ASN	5.3
1	C	199	THR	5.3
1	A	742	TYR	5.3
1	B	102	TYR	5.3
1	C	222	ALA	5.3
1	D	621	PHE	5.3
1	C	689	GLU	5.3
1	C	450	LEU	5.3
1	C	213	PRO	5.3
1	B	504	PRO	5.3
1	A	741	TYR	5.3
1	B	221	VAL	5.3
1	A	216	SER	5.3
1	A	223	MET	5.3
1	A	485	ILE	5.3
1	C	692	GLN	5.3
1	D	168	GLN	5.3
1	A	503	ARG	5.3
1	D	696	ILE	5.3
1	C	295	GLY	5.3
1	A	505	ILE	5.2
1	C	36	ALA	5.2
1	C	315	ARG	5.2
1	D	672	GLY	5.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	502	HIS	5.2
1	A	364	GLY	5.2
1	A	736	LEU	5.2
1	C	31	PRO	5.2
1	D	449	ALA	5.2
1	A	745	THR	5.2
1	C	28	GLY	5.2
1	A	193	MET	5.2
1	B	523	PHE	5.2
1	B	605	PRO	5.2
1	A	645	LEU	5.2
1	D	424	SER	5.2
1	D	446	ALA	5.2
1	B	28	GLY	5.2
1	A	11	GLU	5.2
1	A	608	THR	5.1
1	C	217	SER	5.1
1	D	568	GLY	5.1
1	A	218	CYS	5.1
1	A	82	ALA	5.1
1	A	172	MET	5.1
1	A	648	ASP	5.1
1	A	298	ALA	5.1
1	C	619	GLU	5.1
1	B	580	TYR	5.1
1	D	425	SER	5.1
1	D	194	SER	5.1
1	B	608	THR	5.1
1	A	94	PHE	5.1
1	A	10	LYS	5.1
1	B	156	LEU	5.1
1	B	347	THR	5.1
1	A	214	GLN	5.1
1	C	498	SER	5.1
1	C	620	CYS	5.1
1	B	217	SER	5.0
1	B	289	GLY	5.0
1	D	680	LEU	5.0
1	B	524	ASP	5.0
1	C	626	SER	5.0
1	D	244	THR	5.0
1	A	267	GLY	5.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	186	ALA	5.0
1	B	440	THR	5.0
1	D	175	ALA	5.0
1	C	138	ASP	5.0
1	D	505	ILE	5.0
1	A	417	LYS	5.0
1	B	216	SER	5.0
1	B	174	VAL	5.0
1	A	644	TYR	5.0
1	B	91	THR	5.0
1	A	407	LYS	5.0
1	D	410	CYS	5.0
1	B	451	PRO	5.0
1	D	351	PHE	5.0
1	A	202	SER	5.0
1	D	533	ILE	5.0
1	D	447	SER	5.0
1	B	570	LEU	5.0
1	C	141	PHE	5.0
1	D	325	ALA	5.0
1	A	670	ILE	4.9
1	D	364	GLY	4.9
1	A	693	LYS	4.9
1	D	627	ASN	4.9
1	C	490	TYR	4.9
1	A	597	VAL	4.9
1	D	260	SER	4.9
1	A	248	ILE	4.9
1	C	346	GLY	4.9
1	A	740	MET	4.9
1	A	426	ASN	4.9
1	B	164	ALA	4.9
1	A	491	PRO	4.9
1	B	602	THR	4.9
1	C	604	ALA	4.9
1	A	529	ARG	4.9
1	B	436	ALA	4.9
1	B	384	LYS	4.9
1	C	319	GLY	4.9
1	D	464	THR	4.9
1	A	203	PRO	4.9
1	B	382	THR	4.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	353	PRO	4.9
1	A	621	PHE	4.9
1	D	252	ILE	4.9
1	D	404	VAL	4.9
1	A	562	GLY	4.9
1	A	247	GLY	4.8
1	C	265	THR	4.8
1	A	506	ALA	4.8
1	D	48	TYR	4.8
1	D	482	ASN	4.8
1	C	524	ASP	4.8
1	A	688	TRP	4.8
1	C	168	GLN	4.8
1	B	706	ILE	4.8
1	A	351	PHE	4.8
1	D	40	THR	4.8
1	C	313	ASP	4.8
1	A	432	VAL	4.8
1	C	10	LYS	4.8
1	A	169	HIS	4.8
1	B	144	SER	4.8
1	B	578	LYS	4.8
1	C	360	SER	4.8
1	D	580	TYR	4.8
1	B	741	TYR	4.8
1	A	422	ILE	4.8
1	B	266	ASN	4.8
1	A	669	SER	4.8
1	D	181	ARG	4.7
1	B	540	TYR	4.7
1	B	274	PRO	4.7
1	A	510	GLN	4.7
1	C	225	GLU	4.7
1	C	598	ARG	4.7
1	A	650	VAL	4.7
1	C	124	VAL	4.7
1	D	620	CYS	4.7
1	C	200	HIS	4.7
1	C	499	ASN	4.7
1	D	143	TYR	4.7
1	C	743	LEU	4.7
1	A	522	PRO	4.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	330	PRO	4.7
1	D	328	LEU	4.7
1	A	430	GLU	4.7
1	D	249	GLY	4.7
1	B	202	SER	4.7
1	A	363	TYR	4.7
1	A	5	LYS	4.7
1	C	198	PHE	4.7
1	A	447	SER	4.7
1	D	391	SER	4.7
1	A	123	ILE	4.6
1	A	455	GLU	4.6
1	A	349	THR	4.6
1	B	423	LYS	4.6
1	C	269	SER	4.6
1	D	744	ARG	4.6
1	A	746	GLN	4.6
1	B	109	THR	4.6
1	C	405	VAL	4.6
1	A	301	LEU	4.6
1	A	627	ASN	4.6
1	D	257	SER	4.6
1	C	304	TRP	4.6
1	B	513	ALA	4.6
1	A	87	HIS	4.6
1	C	163	VAL	4.6
1	C	314	ILE	4.6
1	B	245	ALA	4.6
1	A	685	LYS	4.6
1	D	448	VAL	4.6
1	A	306	ALA	4.5
1	C	308	ILE	4.5
1	B	204	THR	4.5
1	D	445	LEU	4.5
1	C	401	THR	4.5
1	C	543	SER	4.5
1	C	603	MET	4.5
1	A	535	ILE	4.5
1	A	561	GLN	4.5
1	B	155	TYR	4.5
1	D	556	PRO	4.5
1	C	669	SER	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	301	LEU	4.5
1	D	138	ASP	4.5
1	C	671	GLN	4.5
1	C	13	VAL	4.5
1	D	69	THR	4.5
1	D	142	GLN	4.5
1	D	185	ALA	4.5
1	D	208	ALA	4.5
1	D	301	LEU	4.5
1	B	610	SER	4.5
1	D	3	VAL	4.5
1	A	560	PHE	4.5
1	B	203	PRO	4.5
1	B	166	ARG	4.5
1	D	452	ALA	4.5
1	A	122	ASN	4.5
1	A	86	LEU	4.5
1	D	608	THR	4.5
1	C	139	ARG	4.5
1	C	45	SER	4.5
1	D	2	TYR	4.4
1	A	268	THR	4.4
1	A	365	ASP	4.4
1	D	263	ALA	4.4
1	D	209	GLY	4.4
1	D	183	ILE	4.4
1	C	49	GLU	4.4
1	A	720	THR	4.4
1	D	248	ILE	4.4
1	D	426	ASN	4.4
1	A	502	HIS	4.4
1	B	215	MET	4.4
1	C	337	LEU	4.4
1	A	91	THR	4.4
1	C	294	PRO	4.4
1	C	35	ASP	4.4
1	A	371	TYR	4.3
1	D	5	LYS	4.3
1	A	702	ARG	4.3
1	C	609	ALA	4.3
1	D	704	VAL	4.3
1	B	137	TYR	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	6	ARG	4.3
1	B	409	ALA	4.3
1	C	502	HIS	4.3
1	D	701	ASP	4.3
1	D	308	ILE	4.3
1	A	401	THR	4.3
1	A	581	GLY	4.3
1	B	342	VAL	4.3
1	D	450	LEU	4.3
1	D	310	ASP	4.3
1	A	418	ASN	4.3
1	D	703	SER	4.3
1	B	214	GLN	4.3
1	B	300	TYR	4.3
1	D	4	TYR	4.3
1	B	168	GLN	4.3
1	C	71	HIS	4.3
1	A	217	SER	4.3
1	B	429	CYS	4.3
1	D	545	GLU	4.2
1	D	650	VAL	4.2
1	A	324	ARG	4.2
1	D	250	LEU	4.2
1	D	317	ASN	4.2
1	D	565	ALA	4.2
1	D	746	GLN	4.2
1	C	157	LEU	4.2
1	D	311	PHE	4.2
1	A	474	ALA	4.2
1	A	578	LYS	4.2
1	A	454	ILE	4.2
1	D	416	GLN	4.2
1	A	651	ASP	4.2
1	A	29	LEU	4.2
1	A	732	TRP	4.2
1	B	383	ILE	4.2
1	C	438	ASP	4.2
1	D	39	VAL	4.2
1	D	178	ILE	4.2
1	B	348	TRP	4.2
1	A	507	LEU	4.2
1	D	743	LEU	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	233	ASP	4.2
1	B	272	LEU	4.2
1	A	201	ALA	4.2
1	C	325	ALA	4.2
1	D	402	PRO	4.2
1	D	628	MET	4.2
1	A	399	THR	4.2
1	B	375	GLU	4.2
1	A	537	GLU	4.1
1	B	271	GLY	4.1
1	A	705	TYR	4.1
1	B	406	TYR	4.1
1	D	716	LEU	4.1
1	B	296	ALA	4.1
1	A	126	GLU	4.1
1	A	200	HIS	4.1
1	A	619	GLU	4.1
1	A	198	PHE	4.1
1	B	420	GLY	4.1
1	D	269	SER	4.1
1	C	201	ALA	4.1
1	B	335	PRO	4.1
1	C	178	ILE	4.1
1	D	180	GLY	4.1
1	D	584	ASP	4.1
1	C	642	ASN	4.1
1	B	341	ARG	4.1
1	B	705	TYR	4.1
1	D	392	ILE	4.1
1	D	485	ILE	4.1
1	A	128	LYS	4.1
1	B	360	SER	4.1
1	A	536	PHE	4.1
1	D	390	TYR	4.1
1	A	355	SER	4.1
1	B	134	ALA	4.0
1	D	677	PRO	4.0
1	B	242	SER	4.0
1	C	607	PRO	4.0
1	D	573	ASP	4.0
1	B	430	GLU	4.0
1	C	379	ARG	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	562	GLY	4.0
1	C	127	ASN	4.0
1	A	209	GLY	4.0
1	A	427	LEU	4.0
1	A	18	ILE	4.0
1	D	697	ASN	4.0
1	A	729	PHE	4.0
1	C	621	PHE	4.0
1	D	361	ASP	4.0
1	D	558	GLU	4.0
1	B	260	SER	4.0
1	D	177	GLY	4.0
1	B	308	ILE	4.0
1	C	714	LEU	4.0
1	D	559	THR	4.0
1	B	176	LEU	4.0
1	C	312	ILE	4.0
1	C	400	GLY	4.0
1	D	65	ALA	4.0
1	B	209	GLY	4.0
1	D	702	ARG	4.0
1	A	175	ALA	4.0
1	A	409	ALA	4.0
1	A	284	ARG	4.0
1	B	303	PRO	4.0
1	B	690	ILE	4.0
1	C	226	ASP	3.9
1	D	1	MET	3.9
1	A	83	ILE	3.9
1	C	474	ALA	3.9
1	B	333	TRP	3.9
1	D	290	GLY	3.9
1	C	627	ASN	3.9
1	B	601	LEU	3.9
1	A	95	SER	3.9
1	A	124	VAL	3.9
1	D	261	TYR	3.9
1	D	388	LEU	3.9
1	A	75	ALA	3.9
1	C	323	ILE	3.9
1	C	167	PRO	3.9
1	C	745	THR	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	297	PHE	3.9
1	A	195	LEU	3.9
1	A	429	CYS	3.9
1	A	317	ASN	3.9
1	C	568	GLY	3.9
1	A	386	GLN	3.9
1	D	546	ALA	3.9
1	C	275	MET	3.9
1	D	544	MET	3.9
1	B	737	LYS	3.8
1	A	531	LEU	3.8
1	B	257	SER	3.8
1	B	463	SER	3.8
1	C	742	TYR	3.8
1	C	19	THR	3.8
1	D	641	VAL	3.8
1	D	557	TYR	3.8
1	B	349	THR	3.8
1	C	102	TYR	3.8
1	C	301	LEU	3.8
1	C	569	ILE	3.8
1	D	267	GLY	3.8
1	C	223	MET	3.8
1	C	473	ILE	3.8
1	A	305	HIS	3.8
1	A	478	THR	3.8
1	A	690	ILE	3.8
1	C	92	LYS	3.8
1	D	225	GLU	3.8
1	A	385	ALA	3.8
1	A	205	LEU	3.8
1	C	717	ARG	3.8
1	C	123	ILE	3.8
1	D	481	LEU	3.8
1	C	562	GLY	3.8
1	D	61	ALA	3.8
1	D	499	ASN	3.8
1	B	606	MET	3.8
1	C	694	THR	3.8
1	D	318	HIS	3.8
1	C	73	ASP	3.8
1	D	512	LEU	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	242	SER	3.8
1	D	642	ASN	3.8
1	B	288	GLN	3.8
1	B	334	ILE	3.8
1	C	342	VAL	3.8
1	C	335	PRO	3.8
1	B	12	PRO	3.8
1	B	307	ASP	3.8
1	B	336	ASP	3.8
1	C	18	ILE	3.8
1	C	567	GLN	3.8
1	B	505	ILE	3.8
1	A	31	PRO	3.7
1	D	434	TYR	3.7
1	C	702	ARG	3.7
1	C	585	TRP	3.7
1	A	368	GLU	3.7
1	D	602	THR	3.7
1	C	69	THR	3.7
1	D	262	ILE	3.7
1	D	41	GLN	3.7
1	B	377	GLU	3.7
1	A	316	LYS	3.7
1	A	708	GLN	3.7
1	B	226	ASP	3.7
1	C	451	PRO	3.7
1	D	706	ILE	3.7
1	A	19	THR	3.7
1	B	573	ASP	3.7
1	C	17	LYS	3.7
1	A	170	LEU	3.7
1	D	206	PHE	3.7
1	B	609	ALA	3.7
1	D	312	ILE	3.7
1	B	667	ASN	3.7
1	A	528	ALA	3.7
1	B	716	LEU	3.7
1	D	205	LEU	3.7
1	D	563	SER	3.7
1	A	545	GLU	3.7
1	A	380	GLY	3.7
1	C	582	MET	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	17	LYS	3.7
1	B	286	VAL	3.7
1	D	411	ASN	3.7
1	B	701	ASP	3.7
1	A	199	THR	3.7
1	B	411	ASN	3.7
1	A	547	SER	3.7
1	A	527	GLU	3.7
1	B	507	LEU	3.7
1	B	3	VAL	3.7
1	B	244	THR	3.7
1	B	353	PRO	3.7
1	A	141	PHE	3.6
1	A	323	ILE	3.6
1	B	490	TYR	3.6
1	D	222	ALA	3.6
1	A	350	LEU	3.6
1	C	737	LYS	3.6
1	B	559	THR	3.6
1	D	11	GLU	3.6
1	C	32	LYS	3.6
1	C	640	VAL	3.6
1	D	210	THR	3.6
1	A	166	ARG	3.6
1	A	384	LYS	3.6
1	C	87	HIS	3.6
1	C	544	MET	3.6
1	D	10	LYS	3.6
1	A	484	VAL	3.6
1	C	570	LEU	3.6
1	D	305	HIS	3.6
1	C	38	LYS	3.6
1	D	281	ASN	3.6
1	D	385	ALA	3.6
1	C	329	PHE	3.6
1	C	531	LEU	3.6
1	D	699	ALA	3.6
1	C	70	VAL	3.6
1	C	117	SER	3.6
1	D	89	GLN	3.6
1	D	223	MET	3.6
1	D	394	GLU	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	36	ALA	3.6
1	C	118	ASP	3.6
1	D	427	LEU	3.5
1	A	465	TYR	3.5
1	B	145	TYR	3.5
1	C	109	THR	3.5
1	A	387	LYS	3.5
1	C	700	ALA	3.5
1	A	28	GLY	3.5
1	D	313	ASP	3.5
1	B	437	PRO	3.5
1	B	717	ARG	3.5
1	B	201	ALA	3.5
1	A	76	THR	3.5
1	B	529	ARG	3.5
1	D	79	ALA	3.5
1	D	639	GLN	3.5
1	B	448	VAL	3.5
1	C	194	SER	3.5
1	B	676	VAL	3.5
1	A	139	ARG	3.5
1	D	298	ALA	3.5
1	D	342	VAL	3.5
1	B	40	THR	3.5
1	A	102	TYR	3.5
1	C	86	LEU	3.5
1	C	250	LEU	3.5
1	D	78	ALA	3.5
1	C	354	THR	3.5
1	A	486	ASP	3.5
1	B	167	PRO	3.5
1	C	103	ARG	3.5
1	A	167	PRO	3.4
1	B	324	ARG	3.4
1	A	397	THR	3.4
1	D	47	VAL	3.4
1	B	205	LEU	3.4
1	D	243	LYS	3.4
1	A	328	LEU	3.4
1	A	603	MET	3.4
1	C	332	LEU	3.4
1	B	337	LEU	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	431	ILE	3.4
1	D	169	HIS	3.4
1	A	677	PRO	3.4
1	D	309	PHE	3.4
1	A	338	PHE	3.4
1	B	577	GLN	3.4
1	B	491	PRO	3.4
1	D	275	MET	3.4
1	A	192	LEU	3.4
1	A	307	ASP	3.4
1	A	234	THR	3.4
1	D	268	THR	3.4
1	D	498	SER	3.4
1	C	707	ASP	3.4
1	A	189	THR	3.4
1	D	307	ASP	3.4
1	A	191	ASN	3.4
1	B	445	LEU	3.4
1	C	40	THR	3.4
1	D	660	LYS	3.4
1	D	728	HIS	3.4
1	A	624	VAL	3.4
1	B	641	VAL	3.4
1	C	34	ILE	3.4
1	C	452	ALA	3.4
1	D	609	ALA	3.4
1	B	70	VAL	3.4
1	A	177	GLY	3.4
1	B	691	SER	3.4
1	C	409	ALA	3.4
1	D	45	SER	3.4
1	B	376	LYS	3.4
1	D	700	ALA	3.4
1	D	71	HIS	3.3
1	D	211	PRO	3.3
1	D	673	LEU	3.3
1	C	72	PRO	3.3
1	B	389	TRP	3.3
1	D	127	ASN	3.3
1	C	387	LYS	3.3
1	D	523	PHE	3.3
1	B	478	THR	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	141	PHE	3.3
1	D	374	TYR	3.3
1	C	122	ASN	3.3
1	D	31	PRO	3.3
1	D	272	LEU	3.3
1	B	584	ASP	3.3
1	D	228	ILE	3.3
1	A	570	LEU	3.3
1	D	363	TYR	3.3
1	D	358	GLY	3.3
1	B	744	ARG	3.3
1	C	701	ASP	3.3
1	D	70	VAL	3.3
1	A	396	GLN	3.3
1	A	431	ILE	3.3
1	B	671	GLN	3.3
1	A	726	SER	3.3
1	A	36	ALA	3.3
1	A	259	GLY	3.3
1	B	206	PHE	3.3
1	C	425	SER	3.3
1	D	534	GLN	3.3
1	D	362	CYS	3.3
1	B	506	ALA	3.3
1	C	331	ALA	3.3
1	D	408	ASP	3.3
1	C	403	PHE	3.3
1	B	739	GLY	3.2
1	D	420	GLY	3.2
1	B	270	ASN	3.2
1	D	535	ILE	3.2
1	D	92	LYS	3.2
1	A	436	ALA	3.2
1	D	9	ARG	3.2
1	A	405	VAL	3.2
1	C	559	THR	3.2
1	B	561	GLN	3.2
1	D	323	ILE	3.2
1	D	338	PHE	3.2
1	B	198	PHE	3.2
1	B	642	ASN	3.2
1	C	37	VAL	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	4	TYR	3.2
1	D	274	PRO	3.2
1	A	410	CYS	3.2
1	D	273	ILE	3.2
1	C	496	ARG	3.2
1	B	746	GLN	3.2
1	C	176	LEU	3.2
1	D	369	ALA	3.2
1	D	401	THR	3.2
1	D	561	GLN	3.2
1	C	309	PHE	3.2
1	D	379	ARG	3.2
1	C	497	LYS	3.2
1	C	685	LYS	3.2
1	C	202	SER	3.2
1	D	271	GLY	3.2
1	B	668	GLY	3.2
1	D	653	GLY	3.2
1	B	419	LEU	3.2
1	B	539	ILE	3.2
1	A	336	ASP	3.2
1	B	745	THR	3.1
1	D	440	THR	3.1
1	C	97	VAL	3.1
1	C	196	LYS	3.1
1	D	280	ASN	3.1
1	D	14	GLN	3.1
1	A	476	VAL	3.1
1	B	139	ARG	3.1
1	D	630	SER	3.1
1	C	437	PRO	3.1
1	C	347	THR	3.1
1	C	597	VAL	3.1
1	D	176	LEU	3.1
1	B	261	TYR	3.1
1	C	326	ARG	3.1
1	A	362	CYS	3.1
1	C	44	ILE	3.1
1	A	180	GLY	3.1
1	D	466	ASN	3.1
1	D	495	ALA	3.1
1	A	297	PHE	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	156	LEU	3.1
1	D	370	LEU	3.1
1	A	135	ILE	3.1
1	C	583	TRP	3.1
1	D	403	PHE	3.1
1	B	558	GLU	3.1
1	C	158	ARG	3.1
1	D	647	ARG	3.1
1	B	240	LEU	3.1
1	D	659	MET	3.1
1	B	108	ALA	3.1
1	B	243	LYS	3.1
1	B	48	TYR	3.1
1	C	126	GLU	3.1
1	C	84	SER	3.1
1	A	9	ARG	3.1
1	A	335	PRO	3.1
1	B	689	GLU	3.1
1	D	365	ASP	3.1
1	D	698	MET	3.1
1	B	688	TRP	3.1
1	C	711	SER	3.0
1	D	229	GLU	3.0
1	A	228	ILE	3.0
1	A	475	LYS	3.0
1	B	39	VAL	3.0
1	B	574	MET	3.0
1	B	612	SER	3.0
1	D	304	TRP	3.0
1	D	629	TYR	3.0
1	D	438	ASP	3.0
1	A	227	SER	3.0
1	C	383	ILE	3.0
1	A	181	ARG	3.0
1	D	157	LEU	3.0
1	D	579	PRO	3.0
1	D	73	ASP	3.0
1	D	386	GLN	3.0
1	A	179	HIS	3.0
1	D	373	ARG	3.0
1	B	462	THR	3.0
1	A	372	THR	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	132	ASN	3.0
1	B	327	ASP	3.0
1	C	311	PHE	3.0
1	B	346	GLY	3.0
1	D	585	TRP	3.0
1	D	324	ARG	3.0
1	D	513	ALA	3.0
1	B	740	MET	3.0
1	B	531	LEU	3.0
1	C	283	ALA	3.0
1	C	355	SER	3.0
1	C	709	SER	3.0
1	D	63	THR	3.0
1	C	169	HIS	3.0
1	A	671	GLN	3.0
1	B	26	CYS	3.0
1	C	76	THR	3.0
1	C	561	GLN	3.0
1	D	51	VAL	2.9
1	B	101	LEU	2.9
1	D	335	PRO	2.9
1	D	400	GLY	2.9
1	A	723	LYS	2.9
1	C	584	ASP	2.9
1	A	367	PHE	2.9
1	B	323	ILE	2.9
1	D	727	MET	2.9
1	A	27	TYR	2.9
1	A	176	LEU	2.9
1	B	306	ALA	2.9
1	C	42	ARG	2.9
1	C	85	ASN	2.9
1	D	483	ARG	2.9
1	C	114	PRO	2.9
1	D	117	SER	2.9
1	A	97	VAL	2.9
1	A	369	ALA	2.9
1	D	381	LYS	2.9
1	C	399	THR	2.9
1	B	528	ALA	2.9
1	B	339	MET	2.9
1	C	361	ASP	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	267	GLY	2.9
1	D	501	ARG	2.9
1	B	338	PHE	2.9
1	C	166	ARG	2.9
1	C	41	GLN	2.9
1	B	173	ARG	2.9
1	D	543	SER	2.9
1	A	314	ILE	2.9
1	C	605	PRO	2.9
1	D	581	GLY	2.9
1	A	538	THR	2.9
1	B	317	ASN	2.9
1	C	119	ASP	2.9
1	B	147	GLY	2.9
1	D	174	VAL	2.9
1	A	721	MET	2.9
1	A	453	PHE	2.8
1	D	7	ASP	2.8
1	D	531	LEU	2.8
1	D	651	ASP	2.8
1	B	312	ILE	2.8
1	D	462	THR	2.8
1	B	388	LEU	2.8
1	D	489	TYR	2.8
1	B	405	VAL	2.8
1	C	121	TYR	2.8
1	C	358	GLY	2.8
1	C	386	GLN	2.8
1	A	701	ASP	2.8
1	B	607	PRO	2.8
1	C	696	ILE	2.8
1	C	419	LEU	2.8
1	A	565	ALA	2.8
1	B	27	TYR	2.8
1	D	241	ILE	2.8
1	C	244	THR	2.8
1	C	356	ALA	2.8
1	A	232	TYR	2.8
1	A	206	PHE	2.8
1	A	596	GLY	2.8
1	A	398	GLU	2.8
1	D	270	ASN	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	480	ASN	2.8
1	A	481	LEU	2.8
1	C	320	LYS	2.8
1	A	40	THR	2.7
1	A	686	THR	2.7
1	B	736	LEU	2.7
1	C	237	GLU	2.7
1	C	408	ASP	2.7
1	A	257	SER	2.7
1	A	23	SER	2.7
1	B	182	ASP	2.7
1	B	185	ALA	2.7
1	D	435	SER	2.7
1	B	142	GLN	2.7
1	D	393	LEU	2.7
1	D	368	GLU	2.7
1	A	649	LEU	2.7
1	C	512	LEU	2.7
1	A	70	VAL	2.7
1	A	196	LYS	2.7
1	A	610	SER	2.7
1	B	157	LEU	2.7
1	A	411	ASN	2.7
1	C	471	HIS	2.7
1	A	235	LEU	2.7
1	C	470	LEU	2.7
1	A	129	ASP	2.7
1	C	300	TYR	2.7
1	D	42	ARG	2.7
1	D	572	PHE	2.7
1	A	84	SER	2.7
1	D	359	LEU	2.7
1	D	640	VAL	2.7
1	C	672	GLY	2.7
1	D	238	CYS	2.7
1	A	121	TYR	2.7
1	A	695	ILE	2.7
1	A	130	LYS	2.7
1	A	273	ILE	2.7
1	B	525	SER	2.7
1	C	181	ARG	2.7
1	C	282	THR	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	609	ALA	2.7
1	A	735	GLY	2.7
1	B	332	LEU	2.7
1	C	310	ASP	2.7
1	D	551	ALA	2.7
1	A	734	LYS	2.7
1	D	314	ILE	2.7
1	A	310	ASP	2.7
1	C	211	PRO	2.7
1	D	646	LEU	2.7
1	C	113	ALA	2.6
1	B	702	ARG	2.6
1	C	639	GLN	2.6
1	A	449	ALA	2.6
1	D	76	THR	2.6
1	B	410	CYS	2.6
1	D	287	ASP	2.6
1	D	300	TYR	2.6
1	D	550	LEU	2.6
1	A	178	ILE	2.6
1	B	422	ILE	2.6
1	B	569	ILE	2.6
1	C	264	GLY	2.6
1	A	501	ARG	2.6
1	B	282	THR	2.6
1	B	427	LEU	2.6
1	D	454	ILE	2.6
1	C	53	THR	2.6
1	C	240	LEU	2.6
1	B	294	PRO	2.6
1	D	322	GLU	2.6
1	B	357	PRO	2.6
1	A	569	ILE	2.6
1	B	374	TYR	2.6
1	B	498	SER	2.6
1	C	566	SER	2.6
1	D	62	GLU	2.6
1	B	482	ASN	2.6
1	B	177	GLY	2.6
1	A	41	GLN	2.6
1	B	352	SER	2.6
1	B	421	VAL	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	743	LEU	2.6
1	C	630	SER	2.6
1	C	6	ARG	2.6
1	A	719	PRO	2.6
1	D	560	PHE	2.6
1	A	65	ALA	2.6
1	B	625	THR	2.6
1	C	68	THR	2.6
1	B	41	GLN	2.6
1	B	503	ARG	2.6
1	B	687	VAL	2.6
1	D	668	GLY	2.6
1	D	336	ASP	2.6
1	C	542	ALA	2.6
1	A	269	SER	2.5
1	B	52	THR	2.5
1	D	306	ALA	2.5
1	D	412	ARG	2.5
1	C	26	CYS	2.5
1	C	39	VAL	2.5
1	A	190	TYR	2.5
1	A	246	GLY	2.5
1	C	316	LYS	2.5
1	B	694	THR	2.5
1	A	118	ASP	2.5
1	A	119	ASP	2.5
1	B	223	MET	2.5
1	D	46	GLY	2.5
1	D	339	MET	2.5
1	A	540	TYR	2.5
1	C	695	ILE	2.5
1	D	68	THR	2.5
1	D	455	GLU	2.5
1	A	155	TYR	2.5
1	A	450	LEU	2.5
1	D	337	LEU	2.5
1	A	539	ILE	2.5
1	B	331	ALA	2.5
1	B	704	VAL	2.5
1	D	618	ASN	2.5
1	B	316	LYS	2.5
1	C	375	GLU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	283	ALA	2.5
1	B	238	CYS	2.5
1	C	381	LYS	2.5
1	C	43	ILE	2.5
1	B	275	MET	2.5
1	B	571	GLN	2.5
1	C	263	ALA	2.5
1	A	618	ASN	2.5
1	A	131	LEU	2.5
1	C	238	CYS	2.5
1	D	38	LYS	2.5
1	D	82	ALA	2.5
1	B	547	SER	2.5
1	B	480	ASN	2.5
1	C	197	TYR	2.5
1	C	698	MET	2.5
1	A	299	LEU	2.5
1	D	343	GLU	2.5
1	C	286	VAL	2.5
1	C	359	LEU	2.5
1	A	103	ARG	2.5
1	B	163	VAL	2.5
1	A	165	GLU	2.4
1	A	402	PRO	2.4
1	B	467	PHE	2.4
1	D	259	GLY	2.4
1	A	563	SER	2.4
1	B	700	ALA	2.4
1	C	511	GLY	2.4
1	D	725	THR	2.4
1	B	325	ALA	2.4
1	C	611	THR	2.4
1	D	330	PRO	2.4
1	A	366	GLU	2.4
1	D	549	GLU	2.4
1	A	271	GLY	2.4
1	C	266	ASN	2.4
1	C	203	PRO	2.4
1	D	367	PHE	2.4
1	C	560	PHE	2.4
1	D	12	PRO	2.4
1	B	439	GLU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	60	ALA	2.4
1	A	244	THR	2.4
1	D	371	TYR	2.4
1	D	619	GLU	2.4
1	C	135	ILE	2.4
1	D	37	VAL	2.4
1	A	89	GLN	2.4
1	B	546	ALA	2.4
1	B	644	TYR	2.4
1	D	654	ILE	2.4
1	C	179	HIS	2.4
1	D	33	HIS	2.4
1	A	551	ALA	2.4
1	D	294	PRO	2.4
1	B	407	LYS	2.4
1	A	464	THR	2.4
1	D	652	LEU	2.4
1	D	603	MET	2.4
1	B	672	GLY	2.4
1	D	29	LEU	2.4
1	B	178	ILE	2.4
1	C	48	TYR	2.4
1	B	356	ALA	2.4
1	C	357	PRO	2.4
1	C	174	VAL	2.4
1	B	169	HIS	2.4
1	C	112	PRO	2.4
1	B	93	GLN	2.4
1	B	549	GLU	2.4
1	B	562	GLY	2.4
1	C	90	THR	2.4
1	B	227	SER	2.4
1	B	269	SER	2.4
1	A	294	PRO	2.4
1	C	699	ALA	2.4
1	A	404	VAL	2.4
1	B	696	ILE	2.3
1	A	463	SER	2.3
1	D	350	LEU	2.3
1	D	731	GLY	2.3
1	C	204	THR	2.3
1	B	34	ILE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	489	TYR	2.3
1	A	347	THR	2.3
1	D	43	ILE	2.3
1	B	544	MET	2.3
1	B	148	PHE	2.3
1	A	238	CYS	2.3
1	D	184	GLU	2.3
1	A	239	ALA	2.3
1	A	283	ALA	2.3
1	C	47	VAL	2.3
1	D	645	LEU	2.3
1	D	465	TYR	2.3
1	B	53	THR	2.3
1	C	276	ILE	2.3
1	D	522	PRO	2.3
1	C	51	VAL	2.3
1	C	175	ALA	2.3
1	C	239	ALA	2.3
1	A	197	TYR	2.3
1	A	628	MET	2.3
1	B	68	THR	2.3
1	D	372	THR	2.3
1	A	270	ASN	2.3
1	B	229	GLU	2.3
1	B	438	ASP	2.3
1	A	718	ALA	2.3
1	B	184	GLU	2.3
1	A	482	ASN	2.3
1	A	689	GLU	2.3
1	B	72	PRO	2.3
1	B	322	GLU	2.3
1	B	453	PHE	2.3
1	C	120	VAL	2.3
1	A	311	PHE	2.3
1	A	356	ALA	2.3
1	A	724	LEU	2.3
1	C	541	HIS	2.3
1	D	655	TRP	2.3
1	A	361	ASP	2.3
1	A	388	LEU	2.3
1	B	479	ARG	2.3
1	D	77	LEU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	241	ILE	2.2
1	D	334	ILE	2.2
1	A	678	GLN	2.2
1	D	332	LEU	2.2
1	D	341	ARG	2.2
1	A	274	PRO	2.2
1	A	287	ASP	2.2
1	B	514	ASP	2.2
1	B	543	SER	2.2
1	D	64	CYS	2.2
1	A	330	PRO	2.2
1	A	224	LYS	2.2
1	D	574	MET	2.2
1	D	675	ASN	2.2
1	A	44	ILE	2.2
1	A	389	TRP	2.2
1	D	329	PHE	2.2
1	B	695	ILE	2.2
1	A	39	VAL	2.2
1	A	414	SER	2.2
1	D	66	TYR	2.2
1	C	260	SER	2.2
1	D	726	SER	2.2
1	A	210	THR	2.2
1	A	26	CYS	2.2
1	B	685	LYS	2.2
1	D	492	VAL	2.2
1	A	53	THR	2.2
1	A	611	THR	2.2
1	B	69	THR	2.2
1	C	27	TYR	2.2
1	A	289	GLY	2.2
1	B	290	GLY	2.2
1	D	8	GLY	2.2
1	C	83	ILE	2.2
1	B	258	THR	2.2
1	A	348	TRP	2.2
1	B	692	GLN	2.2
1	A	22	ILE	2.2
1	C	344	GLU	2.2
1	C	727	MET	2.2
1	C	697	ASN	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	74	TYR	2.2
1	B	350	LEU	2.2
1	D	35	ASP	2.2
1	A	186	ALA	2.2
1	B	124	VAL	2.1
1	D	44	ILE	2.1
1	D	662	TYR	2.1
1	D	163	VAL	2.1
1	A	242	SER	2.1
1	B	428	CYS	2.1
1	A	236	LYS	2.1
1	A	79	ALA	2.1
1	D	315	ARG	2.1
1	B	110	GLY	2.1
1	B	239	ALA	2.1
1	D	409	ALA	2.1
1	B	408	ASP	2.1
1	A	511	GLY	2.1
1	B	663	LEU	2.1
1	C	209	GLY	2.1
1	C	284	ARG	2.1
1	A	492	VAL	2.1
1	B	486	ASP	2.1
1	D	507	LEU	2.1
1	A	57	ASP	2.1
1	A	370	LEU	2.1
1	A	120	VAL	2.1
1	D	375	GLU	2.1
1	C	523	PHE	2.1
1	A	272	LEU	2.1
1	C	667	ASN	2.1
1	A	333	TRP	2.1
1	A	88	LYS	2.1
1	B	285	TYR	2.1
1	B	340	LYS	2.1
1	B	107	ALA	2.1
1	B	598	ARG	2.1
1	C	125	MET	2.1
1	C	188	GLU	2.1
1	B	90	THR	2.1
1	B	565	ALA	2.1
1	B	186	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	452	ALA	2.1
1	B	495	ALA	2.1
1	D	349	THR	2.1
1	D	592	ILE	2.1
1	D	170	LEU	2.1
1	D	384	LYS	2.1
1	B	502	HIS	2.1
1	D	736	LEU	2.1
1	D	124	VAL	2.1
1	D	453	PHE	2.1
1	A	226	ASP	2.0
1	B	485	ILE	2.0
1	D	16	ASP	2.0
1	D	21	ARG	2.0
1	D	75	ALA	2.0
1	C	321	GLU	2.0
1	D	100	ASP	2.0
1	A	67	MET	2.0
1	A	213	PRO	2.0
1	C	334	ILE	2.0
1	B	648	ASP	2.0
1	B	614	ILE	2.0
1	D	656	ASP	2.0
1	B	262	ILE	2.0
1	A	379	ARG	2.0
1	B	361	ASP	2.0
1	A	81	ILE	2.0
1	D	299	LEU	2.0
1	B	232	TYR	2.0
1	D	437	PRO	2.0
1	B	386	GLN	2.0

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 [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.