



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 01:57 AM UTC

PDB ID : 4V4Q / pdb_00004v4q
Title : Crystal structure of the bacterial ribosome from Escherichia coli at 3.5 Å resolution.
Authors : Schuwirth, B.S.; Borovinskaya, M.A.; Hau, C.W.; Zhang, W.; Vila-Sanjurjo, A.; Holton, J.M.; Cate, J.H.D.
Deposited on : 2005-08-30
Resolution : 3.46 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	FAILED
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.48.1

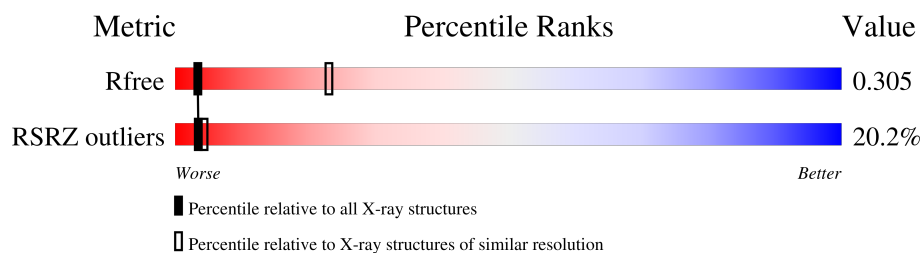
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.46 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}	164625	1597 (3.52-3.40)
RSRZ outliers	164620	1596 (3.52-3.40)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 54 unique types of molecules in this entry. The entry contains 284107 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 RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1530	Total	C	N	O	P	0	0	0
			32831	14642	6024	10635	1530			
1	CA	1530	Total	C	N	O	P	0	0	0
			32831	14642	6024	10635	1530			

- Molecule 2 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AC	206	Total	C	N	O	S	0	0	0
			1624	1028	305	288	3			
2	CC	206	Total	C	N	O	S	0	0	0
			1624	1028	305	288	3			

- Molecule 3 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AD	205	Total	C	N	O	S	0	0	0
			1643	1026	315	298	4			
3	CD	205	Total	C	N	O	S	0	0	0
			1643	1026	315	298	4			

- Molecule 4 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AE	150	Total	C	N	O	S	0	0	0
			1105	687	211	201	6			
4	CE	150	Total	C	N	O	S	0	0	0
			1105	687	211	201	6			

- Molecule 5 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AF	100	Total	C	N	O	S	0	0	0
			817	515	148	148	6			
5	CF	100	Total	C	N	O	S	0	0	0
			817	515	148	148	6			

- Molecule 6 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AG	150	Total	C	N	O	S	0	0	0
			1174	730	226	214	4			
6	CG	152	Total	C	N	O	S	0	0	0
			1196	745	230	217	4			

- Molecule 7 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			
7	CH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			

- Molecule 8 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AI	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			
8	CI	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			

- Molecule 9 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AJ	98	Total	C	N	O	S	0	0	0
			786	493	150	142	1			
9	CJ	98	Total	C	N	O	S	0	0	0
			786	493	150	142	1			

- Molecule 10 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AK	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	CK	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			

- Molecule 11 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AL	123	Total	C	N	O	S	0	0	0
			955	590	196	165	4			
11	CL	123	Total	C	N	O	S	0	0	0
			955	590	196	165	4			

- Molecule 12 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AM	114	Total	C	N	O	S	0	0	0
			883	546	178	156	3			
12	CM	113	Total	C	N	O	S	0	0	0
			876	541	177	155	3			

- Molecule 13 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AN	96	Total	C	N	O	S	0	0	0
			774	483	160	128	3			
13	CN	96	Total	C	N	O	S	0	0	0
			774	483	160	128	3			

- Molecule 14 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AO	88	Total	C	N	O	S	0	0	0
			716	440	146	129	1			
14	CO	88	Total	C	N	O	S	0	0	0
			716	440	146	129	1			

- Molecule 15 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			
15	CP	80	Total	C	N	O	S	0	0	0
			638	400	126	111	1			

- Molecule 16 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AQ	80	Total	C	N	O	S	0	0	0
			648	411	121	113	3			
16	CQ	81	Total	C	N	O	S	0	0	0
			656	417	122	114	3			

- Molecule 17 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	AR	55	Total	C	N	O	0	0	0
			455	288	86	81			
17	CR	55	Total	C	N	O	0	0	0
			455	288	86	81			

- Molecule 18 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AS	79	Total	C	N	O	S	0	0	0
			637	408	120	107	2			
18	CS	80	Total	C	N	O	S	0	0	0
			644	413	121	108	2			

- Molecule 19 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AT	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			
19	CT	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			

- Molecule 20 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AB	218	Total	C	N	O	S	0	0	0
			1704	1081	305	311	7			
20	CB	218	Total	C	N	O	S	0	0	0
			1704	1081	305	311	7			

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AU	51	Total	C	N	O	S	0	0	0
			425	265	86	73	1			
21	CU	51	Total	C	N	O	S	0	0	0
			425	265	86	73	1			

- Molecule 22 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	BA	117	Total	C	N	O	P	0	0	0
			2507	1116	459	815	117			
22	DA	117	Total	C	N	O	P	0	0	0
			2507	1116	459	815	117			

- Molecule 23 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	BB	2841	Total	C	N	O	P	0	0	0
			60995	27210	11229	19715	2841			
23	DB	2841	Total	C	N	O	P	0	0	0
			60995	27210	11229	19715	2841			

- Molecule 24 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	BV	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			
24	DV	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			

- Molecule 25 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BC	267	Total	C	N	O	S	0	0	0
			2053	1271	416	359	7			
25	DC	267	Total	C	N	O	S	0	0	0
			2053	1271	416	359	7			

- Molecule 26 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BD	209	Total	C	N	O	S	0	0	0
			1565	979	288	294	4			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	DD	209	Total	C	N	O	S	0	0	0
			1565	979	288	294	4			

- Molecule 27 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BE	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			
27	DE	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			

- Molecule 28 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BF	178	Total	C	N	O	S	0	0	0
			1420	905	251	258	6			
28	DF	178	Total	C	N	O	S	0	0	0
			1420	905	251	258	6			

- Molecule 29 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BG	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			
29	DG	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			

- Molecule 30 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BH	149	Total	C	N	O	S	0	0	0
			1111	699	197	214	1			
30	DH	149	Total	C	N	O	S	0	0	0
			1111	699	197	214	1			

- Molecule 31 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BJ	140	Total	C	N	O	S	0	0	0
			1112	704	210	194	4			
31	DJ	140	Total	C	N	O	S	0	0	0
			1112	704	210	194	4			

- Molecule 32 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BK	121	Total	C	N	O	S	0	0	0
			930	582	179	164	5			
32	DK	121	Total	C	N	O	S	0	0	0
			930	582	179	164	5			

- Molecule 33 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BL	144	Total	C	N	O	S	0	0	0
			1053	654	207	190	2			
33	DL	144	Total	C	N	O	S	0	0	0
			1053	654	207	190	2			

- Molecule 34 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BM	136	Total	C	N	O	S	0	0	0
			1074	686	205	177	6			
34	DM	136	Total	C	N	O	S	0	0	0
			1074	686	205	177	6			

- Molecule 35 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BN	127	Total	C	N	O	S	0	0	0
			1008	621	204	178	5			
35	DN	127	Total	C	N	O	S	0	0	0
			1008	621	204	178	5			

- Molecule 36 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BO	117	Total	C	N	O	S	0	0	0
			900	557	179	163	1			
36	DO	117	Total	C	N	O	S	0	0	0
			900	557	179	163	1			

- Molecule 37 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BP	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			
37	DP	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			

- Molecule 38 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BQ	117	Total	C	N	O	S	0	0	0
			947	604	192	151				
38	DQ	117	Total	C	N	O	S	0	0	0
			947	604	192	151				

- Molecule 39 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BR	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			
39	DR	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			

- Molecule 40 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BS	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			
40	DS	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			

- Molecule 41 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BT	99	Total	C	N	O	S	0	0	0
			777	491	145	139	2			
41	DT	99	Total	C	N	O	S	0	0	0
			777	491	145	139	2			

- Molecule 42 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BU	102	Total	C	N	O	S	0	0	0
			779	492	146	141				

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
42	DU	102	Total	C	N	O			
			779	492	146	141	0	0	0

- Molecule 43 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
43	BW	84	Total	C	N	O	S		
			634	391	129	113	1	0	0
43	DW	84	Total	C	N	O	S		
			634	391	129	113	1	0	0

- Molecule 44 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
44	BX	63	Total	C	N	O	S		
			509	313	99	95	2	0	0
44	DX	63	Total	C	N	O	S		
			509	313	99	95	2	0	0

- Molecule 45 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
45	BY	58	Total	C	N	O	S		
			449	281	87	79	2	0	0
45	DY	58	Total	C	N	O	S		
			449	281	87	79	2	0	0

- Molecule 46 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
46	BZ	70	Total	C	N	O	S		
			549	339	104	100	6	0	0
46	DZ	70	Total	C	N	O	S		
			549	339	104	100	6	0	0

- Molecule 47 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
47	B0	56	Total	C	N	O	S		
			444	269	94	80	1	0	0
47	D0	56	Total	C	N	O	S		
			444	269	94	80	1	0	0

- Molecule 48 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
48	B1	54	Total	C	N	O	0	0	0
			441	284	81	76			
48	D1	54	Total	C	N	O	0	0	0
			441	284	81	76			

- Molecule 49 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	B2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			
49	D2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			

- Molecule 50 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			
50	D3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			

- Molecule 51 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			
51	D4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			

- Molecule 52 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	BI	141	Total	C	N	O	S	0	0	0
			1032	651	179	196	6			
52	DI	141	Total	C	N	O	S	0	0	0
			1032	651	179	196	6			

- Molecule 53 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
53	AA	59	Total Mg 59 59	0	0
53	AP	1	Total Mg 1 1	0	0
53	BB	110	Total Mg 110 110	0	0
53	CA	62	Total Mg 62 62	0	0
53	DB	110	Total Mg 110 110	0	0
53	DN	1	Total Mg 1 1	0	0

- Molecule 54 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
54	AA	290	Total O 290 290	0	0
54	AE	3	Total O 3 3	0	0
54	AK	2	Total O 2 2	0	0
54	AN	4	Total O 4 4	0	0
54	AP	1	Total O 1 1	0	0
54	BB	497	Total O 497 497	0	0
54	BC	1	Total O 1 1	0	0
54	BE	5	Total O 5 5	0	0
54	BH	1	Total O 1 1	0	0
54	BL	2	Total O 2 2	0	0
54	BN	1	Total O 1 1	0	0
54	CA	295	Total O 295 295	0	0
54	CE	3	Total O 3 3	0	0
54	CK	1	Total O 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	CL	4	Total 4	O 4	0	0
54	CN	2	Total 2	O 2	0	0
54	CP	1	Total 1	O 1	0	0
54	CT	2	Total 2	O 2	0	0
54	DB	499	Total 499	O 499	0	0
54	DC	1	Total 1	O 1	0	0
54	DD	1	Total 1	O 1	0	0
54	DE	3	Total 3	O 3	0	0
54	DJ	2	Total 2	O 2	0	0
54	DL	1	Total 1	O 1	0	0
54	DN	2	Total 2	O 2	0	0
54	DQ	1	Total 1	O 1	0	0
54	D2	2	Total 2	O 2	0	0

MolProbity failed to run properly - this section is therefore empty.

3 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	208.85Å 379.20Å 739.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.00 – 3.46 70.00 – 3.46	Depositor EDS
% Data completeness (in resolution range)	91.6 (70.00-3.46) 91.5 (70.00-3.46)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 3.49Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.279 , 0.331 0.261 , 0.305	Depositor DCC
R_{free} test set	35586 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	77.0	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 66.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	284107	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.43% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 343 ligands modelled in this entry, 343 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
21	AU	2
21	CU	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	CU	25:ALA	C	26:GLY	N	1.60
1	AU	25:ALA	C	26:GLY	N	1.16
1	AU	15:LEU	C	16:ARG	N	0.99

5 Fit of model and data ⓘ

5.1 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	AA	1530/1542 (99%)	0.72	98 (6%) 27 22	16, 66, 135, 180	0
1	CA	1530/1542 (99%)	0.40	63 (4%) 42 31	11, 49, 119, 180	0
2	AC	206/232 (88%)	0.66	18 (8%) 17 15	8, 56, 116, 163	0
2	CC	206/232 (88%)	0.79	22 (10%) 12 12	13, 68, 122, 154	0
3	AD	205/205 (100%)	1.15	45 (21%) 3 4	16, 65, 125, 180	0
3	CD	205/205 (100%)	0.69	20 (9%) 14 13	5, 49, 103, 156	0
4	AE	150/166 (90%)	0.78	11 (7%) 22 19	5, 56, 104, 151	0
4	CE	150/166 (90%)	0.52	13 (8%) 17 15	5, 49, 101, 167	0
5	AF	100/135 (74%)	0.73	8 (8%) 20 17	19, 64, 113, 150	0
5	CF	100/135 (74%)	1.04	18 (18%) 4 5	10, 65, 113, 147	0
6	AG	150/178 (84%)	1.03	25 (16%) 5 6	23, 86, 133, 180	0
6	CG	152/178 (85%)	0.86	17 (11%) 11 11	22, 83, 132, 166	0
7	AH	129/129 (100%)	0.87	16 (12%) 9 9	8, 63, 113, 155	0
7	CH	129/129 (100%)	0.82	14 (10%) 12 12	5, 49, 104, 154	0
8	AI	127/129 (98%)	1.16	23 (18%) 4 5	5, 83, 126, 169	0
8	CI	127/129 (98%)	1.41	31 (24%) 2 3	22, 81, 135, 161	0
9	AJ	98/103 (95%)	1.23	18 (18%) 4 5	14, 76, 141, 160	0
9	CJ	98/103 (95%)	1.23	21 (21%) 3 4	27, 78, 122, 143	0
10	AK	117/128 (91%)	0.94	15 (12%) 9 9	6, 56, 99, 164	0
10	CK	117/128 (91%)	0.63	9 (7%) 21 18	5, 44, 95, 117	0
11	AL	123/123 (100%)	1.23	30 (24%) 2 3	18, 59, 115, 162	0
11	CL	123/123 (100%)	0.68	18 (14%) 7 8	5, 34, 109, 141	0
12	AM	114/117 (97%)	1.28	25 (21%) 3 4	37, 96, 137, 155	0
12	CM	113/117 (96%)	1.20	21 (18%) 4 5	19, 92, 143, 180	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AN	96/100 (96%)	1.40	31 (32%) 1 2	11, 76, 133, 147	0
13	CN	96/100 (96%)	1.31	26 (27%) 2 3	32, 73, 130, 160	0
14	AO	88/89 (98%)	0.80	11 (12%) 9 9	15, 62, 104, 177	0
14	CO	88/89 (98%)	0.73	9 (10%) 13 12	5, 46, 113, 136	0
15	AP	82/82 (100%)	1.27	21 (25%) 2 3	20, 72, 132, 171	0
15	CP	80/82 (97%)	1.01	12 (15%) 6 7	5, 42, 126, 137	0
16	AQ	80/83 (96%)	1.08	14 (17%) 5 6	34, 77, 119, 158	0
16	CQ	81/83 (97%)	0.95	14 (17%) 5 6	11, 52, 113, 155	0
17	AR	55/74 (74%)	1.02	9 (16%) 5 6	16, 60, 124, 148	0
17	CR	55/74 (74%)	0.75	7 (12%) 9 9	17, 45, 118, 139	0
18	AS	79/91 (86%)	1.39	20 (25%) 2 3	44, 110, 140, 169	0
18	CS	80/91 (87%)	1.55	22 (27%) 2 2	47, 99, 151, 161	0
19	AT	85/86 (98%)	1.21	18 (21%) 3 4	37, 83, 123, 155	0
19	CT	85/86 (98%)	1.00	13 (15%) 6 7	9, 49, 103, 138	0
20	AB	218/240 (90%)	0.90	33 (15%) 6 7	17, 82, 131, 156	0
20	CB	218/240 (90%)	0.94	34 (15%) 6 7	13, 90, 135, 162	0
21	AU	51/71 (71%)	1.56	15 (29%) 1 2	29, 80, 131, 158	0
21	CU	51/71 (71%)	1.86	20 (39%) 1 1	34, 73, 112, 140	0
22	BA	117/120 (97%)	0.48	8 (6%) 25 21	36, 62, 94, 157	0
22	DA	117/120 (97%)	0.90	9 (7%) 21 18	27, 62, 113, 180	0
23	BB	2841/2904 (97%)	0.55	177 (6%) 28 23	10, 49, 134, 180	0
23	DB	2841/2904 (97%)	0.38	140 (4%) 36 27	5, 39, 133, 180	0
24	BV	94/94 (100%)	0.83	12 (12%) 9 9	20, 75, 130, 149	0
24	DV	94/94 (100%)	0.95	12 (12%) 9 9	17, 71, 119, 130	0
25	BC	267/273 (97%)	1.98	104 (38%) 1 1	5, 51, 136, 180	0
25	DC	267/273 (97%)	2.21	120 (44%) 1 0	5, 46, 139, 180	0
26	BD	209/209 (100%)	2.75	104 (49%) 0 0	21, 82, 174, 180	0
26	DD	209/209 (100%)	2.14	96 (45%) 1 0	5, 60, 139, 180	0
27	BE	201/201 (100%)	2.32	103 (51%) 0 0	8, 78, 147, 180	0
27	DE	201/201 (100%)	2.31	98 (48%) 0 0	5, 76, 164, 180	0
28	BF	178/178 (100%)	1.33	41 (23%) 2 3	43, 98, 152, 180	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
28	DF	178/178 (100%)	1.41	51 (28%)	1	2	29, 89, 138, 180	0
29	BG	176/176 (100%)	1.38	38 (21%)	3	4	23, 94, 154, 180	0
29	DG	176/176 (100%)	1.28	41 (23%)	2	3	20, 86, 154, 172	0
30	BH	149/149 (100%)	1.51	41 (27%)	2	2	23, 120, 170, 180	0
30	DH	149/149 (100%)	1.59	49 (32%)	1	2	31, 100, 153, 180	0
31	BJ	140/142 (98%)	2.25	63 (45%)	1	0	14, 79, 160, 180	0
31	DJ	140/142 (98%)	2.18	66 (47%)	0	0	14, 61, 136, 162	0
32	BK	121/123 (98%)	1.11	24 (19%)	3	4	13, 57, 106, 147	0
32	DK	121/123 (98%)	0.89	15 (12%)	9	9	5, 37, 84, 143	0
33	BL	144/144 (100%)	3.72	100 (69%)	0	0	19, 93, 160, 180	0
33	DL	144/144 (100%)	2.89	79 (54%)	0	0	7, 74, 150, 179	0
34	BM	136/136 (100%)	2.48	74 (54%)	0	0	16, 71, 168, 180	0
34	DM	136/136 (100%)	2.17	66 (48%)	0	0	10, 66, 152, 180	0
35	BN	127/127 (100%)	2.27	56 (44%)	1	0	19, 67, 149, 180	0
35	DN	127/127 (100%)	1.50	37 (29%)	1	2	5, 45, 143, 180	0
36	BO	117/117 (100%)	2.48	59 (50%)	0	0	20, 82, 150, 180	0
36	DO	117/117 (100%)	2.09	58 (49%)	0	0	20, 77, 150, 169	0
37	BP	114/114 (100%)	1.99	50 (43%)	1	0	21, 84, 177, 180	0
37	DP	114/114 (100%)	2.53	60 (52%)	0	0	8, 69, 148, 180	0
38	BQ	117/117 (100%)	1.77	43 (36%)	1	1	8, 63, 125, 174	0
38	DQ	117/117 (100%)	2.07	53 (45%)	1	0	11, 57, 127, 180	0
39	BR	103/103 (100%)	2.79	59 (57%)	0	0	33, 100, 153, 180	0
39	DR	103/103 (100%)	2.82	56 (54%)	0	0	26, 92, 154, 180	0
40	BS	110/110 (100%)	1.66	31 (28%)	1	2	14, 57, 132, 180	0
40	DS	110/110 (100%)	1.21	27 (24%)	2	3	5, 45, 137, 175	0
41	BT	99/100 (99%)	1.82	37 (37%)	1	1	25, 73, 150, 170	0
41	DT	99/100 (99%)	1.81	40 (40%)	1	1	16, 84, 160, 180	0
42	BU	102/103 (99%)	2.61	50 (49%)	0	0	18, 92, 158, 178	0
42	DU	102/103 (99%)	2.89	61 (59%)	0	0	11, 103, 161, 180	0
43	BW	84/84 (100%)	3.20	57 (67%)	0	0	22, 87, 153, 180	0
43	DW	84/84 (100%)	3.19	54 (64%)	0	0	20, 81, 149, 180	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
44	BX	63/63 (100%)	1.51	19 (30%)	1	2	28, 92, 148, 170	0
44	DX	63/63 (100%)	2.40	30 (47%)	0	0	47, 96, 162, 171	0
45	BY	58/58 (100%)	2.20	26 (44%)	1	0	29, 72, 150, 180	0
45	DY	58/58 (100%)	1.56	16 (27%)	2	2	5, 60, 129, 177	0
46	BZ	70/70 (100%)	2.69	38 (54%)	0	0	20, 68, 134, 168	0
46	DZ	70/70 (100%)	3.12	47 (67%)	0	0	16, 59, 132, 180	0
47	B0	56/56 (100%)	3.02	38 (67%)	0	0	23, 89, 163, 180	0
47	D0	56/56 (100%)	2.24	24 (42%)	1	1	12, 61, 148, 180	0
48	B1	54/54 (100%)	1.58	17 (31%)	1	2	18, 89, 142, 179	0
48	D1	54/54 (100%)	2.06	22 (40%)	1	1	22, 77, 153, 173	0
49	B2	46/46 (100%)	2.21	19 (41%)	1	1	11, 47, 152, 180	0
49	D2	46/46 (100%)	2.31	25 (54%)	0	0	13, 48, 112, 129	0
50	B3	64/64 (100%)	2.89	32 (50%)	0	0	15, 61, 149, 180	0
50	D3	64/64 (100%)	2.83	34 (53%)	0	0	8, 55, 125, 169	0
51	B4	38/38 (100%)	3.43	28 (73%)	0	0	36, 85, 161, 180	0
51	D4	38/38 (100%)	4.56	34 (89%)	0	0	20, 80, 168, 180	0
52	BI	141/141 (100%)	2.24	78 (55%)	0	0	61, 151, 180, 180	0
52	DI	141/141 (100%)	1.85	57 (40%)	1	1	84, 157, 180, 180	0
All	All	20439/21034 (97%)	1.15	4131 (20%)	3	4	5, 61, 145, 180	0

All (4131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
42	BU	29	SER	15.0
45	BY	3	THR	14.8
26	BD	134	HIS	13.6
42	BU	89	GLY	13.0
33	BL	82	LEU	12.9
27	DE	3	LEU	12.7
26	BD	132	ALA	12.2
33	BL	34	GLY	11.9
51	B4	23	ILE	11.9
39	DR	53	PHE	11.8
37	DP	80	VAL	11.5
46	DZ	4	ASP	11.4
23	DB	2133	G	11.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
43	BW	68	PHE	11.3
50	B3	23	HIS	11.2
42	DU	2	ALA	11.1
26	BD	133	THR	10.9
29	BG	1	SER	10.8
25	BC	241	LYS	10.8
33	BL	38	GLN	10.6
25	DC	209	ALA	10.4
42	DU	27	VAL	10.4
26	BD	140	HIS	10.4
51	D4	7	VAL	10.3
43	DW	37	VAL	10.3
33	DL	99	ASN	10.0
26	BD	135	GLY	9.9
33	BL	53	GLY	9.9
33	BL	35	HIS	9.9
34	BM	92	TRP	9.8
33	BL	58	TYR	9.8
33	DL	55	MET	9.8
33	BL	25	SER	9.8
50	D3	35	LYS	9.6
51	D4	31	PRO	9.6
25	BC	239	PHE	9.6
43	BW	45	HIS	9.6
25	DC	178	GLY	9.6
33	DL	52	GLY	9.6
39	DR	12	HIS	9.5
35	BN	67	PHE	9.5
33	BL	37	GLY	9.5
46	BZ	22	MET	9.5
43	BW	69	GLU	9.5
33	BL	39	LYS	9.5
40	BS	103	ILE	9.4
47	B0	8	THR	9.4
43	DW	68	PHE	9.4
27	BE	201	ALA	9.4
33	BL	46	VAL	9.4
43	BW	37	VAL	9.4
51	B4	7	VAL	9.4
33	BL	66	PHE	9.3
26	BD	139	SER	9.3
49	B2	1	MET	9.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
36	BO	59	ALA	9.3
27	DE	171	ASP	9.2
42	BU	28	LEU	9.2
33	BL	40	SER	9.2
26	BD	153	GLY	9.2
31	DJ	46	PRO	9.1
36	BO	57	ALA	9.1
34	DM	24	THR	9.0
33	BL	99	ASN	9.0
51	D4	1	MET	9.0
34	DM	91	TYR	8.9
23	DB	2402	U	8.9
30	DH	122	LEU	8.9
38	BQ	111	LYS	8.8
37	DP	59	THR	8.8
47	D0	48	TYR	8.8
51	D4	23	ILE	8.8
50	D3	33	THR	8.8
25	BC	224	MET	8.7
18	CS	78	THR	8.7
43	BW	52	CYS	8.7
46	DZ	18	CYS	8.6
26	BD	152	PRO	8.6
26	BD	150	GLN	8.6
33	DL	100	ILE	8.5
25	DC	218	THR	8.5
39	DR	44	GLY	8.5
50	B3	63	TYR	8.4
25	BC	218	THR	8.4
50	D3	32	LEU	8.4
37	BP	97	TYR	8.4
43	DW	58	LEU	8.4
26	BD	148	GLN	8.4
25	DC	247	TRP	8.3
25	DC	244	VAL	8.3
35	BN	112	TYR	8.3
26	BD	149	ASN	8.3
25	DC	242	HIS	8.2
33	BL	56	PRO	8.2
35	BN	20	MET	8.2
43	BW	36	ILE	8.2
25	BC	85	ASN	8.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
35	BN	3	HIS	8.2
25	BC	242	HIS	8.2
31	BJ	79	GLY	8.1
38	BQ	88	GLU	8.1
33	BL	67	THR	8.1
23	BB	2145	C	8.1
51	D4	37	GLN	8.1
33	BL	52	GLY	8.0
38	BQ	90	ASP	8.0
26	BD	127	PHE	8.0
39	DR	83	TYR	8.0
29	BG	58	ALA	8.0
16	AQ	4	ILE	8.0
27	BE	104	ALA	8.0
39	BR	52	PRO	8.0
43	BW	19	ARG	7.9
43	DW	25	PHE	7.9
3	AD	3	TYR	7.9
51	D4	38	GLY	7.8
39	BR	43	ASN	7.8
50	D3	28	LEU	7.8
46	BZ	63	ARG	7.8
40	BS	10	ALA	7.8
25	DC	85	ASN	7.8
33	BL	83	ALA	7.7
25	BC	247	TRP	7.7
50	B3	28	LEU	7.7
23	BB	2308	G	7.7
31	DJ	49	ASP	7.7
26	BD	147	GLY	7.7
33	DL	59	ARG	7.7
38	DQ	96	ASP	7.6
31	DJ	50	THR	7.6
33	BL	77	ILE	7.6
38	DQ	46	TYR	7.6
46	DZ	48	GLN	7.6
26	DD	33	ARG	7.6
18	CS	1	PRO	7.6
29	BG	51	PHE	7.6
39	BR	54	VAL	7.6
36	BO	58	ILE	7.6
50	B3	57	VAL	7.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	BK	67	LYS	7.5
26	DD	49	GLN	7.5
39	DR	43	ASN	7.5
39	DR	87	GLN	7.5
42	BU	61	GLU	7.5
31	BJ	47	HIS	7.5
33	BL	54	GLN	7.5
49	B2	14	ARG	7.5
33	DL	97	ALA	7.5
39	DR	42	ALA	7.5
36	DO	66	GLY	7.4
34	BM	26	VAL	7.4
49	B2	18	PHE	7.4
17	AR	63	TYR	7.4
42	BU	1	ALA	7.4
46	BZ	27	THR	7.3
37	DP	97	TYR	7.3
42	BU	2	ALA	7.3
31	BJ	89	PHE	7.3
47	B0	34	GLY	7.3
39	DR	5	PHE	7.3
22	DA	28	C	7.2
25	BC	209	ALA	7.2
46	BZ	56	ARG	7.2
36	BO	8	ILE	7.2
51	B4	1	MET	7.2
33	DL	73	ILE	7.2
42	BU	30	SER	7.2
50	B3	61	LEU	7.2
42	DU	81	ARG	7.2
42	DU	44	HIS	7.2
25	BC	268	ARG	7.2
26	BD	130	GLN	7.2
31	BJ	10	THR	7.2
31	DJ	102	GLU	7.2
37	BP	13	LYS	7.1
26	BD	126	ASN	7.1
26	BD	141	ARG	7.1
37	DP	113	LEU	7.1
25	DC	239	PHE	7.1
47	B0	7	PRO	7.1
25	DC	241	LYS	7.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
46	DZ	9	TYR	7.0
13	AN	1	ALA	7.0
36	BO	97	PHE	7.0
25	BC	41	GLY	7.0
26	DD	17	GLU	7.0
39	BR	78	ARG	7.0
10	AK	118	ASN	7.0
30	DH	25	TYR	7.0
47	B0	6	LYS	7.0
26	DD	127	PHE	6.9
8	CI	127	SER	6.9
27	BE	4	VAL	6.9
26	DD	2	ILE	6.9
37	DP	55	HIS	6.9
51	D4	21	GLY	6.9
50	B3	29	ARG	6.9
31	BJ	48	VAL	6.9
8	CI	129	ARG	6.9
29	BG	61	TRP	6.9
26	BD	129	THR	6.9
36	BO	56	LYS	6.8
43	DW	3	LYS	6.8
33	BL	57	LEU	6.8
34	BM	64	TRP	6.8
27	DE	84	THR	6.8
10	CK	128	VAL	6.8
26	DD	51	THR	6.8
33	DL	12	SER	6.8
42	BU	32	LYS	6.8
42	DU	92	VAL	6.8
23	BB	645	C	6.8
39	BR	86	GLN	6.8
23	BB	2309	A	6.8
27	DE	48	THR	6.7
37	BP	59	THR	6.7
50	B3	26	ALA	6.7
33	BL	19	LEU	6.7
45	BY	13	ILE	6.7
29	DG	1	SER	6.7
33	DL	25	SER	6.7
44	DX	46	VAL	6.7
33	DL	35	HIS	6.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
36	DO	59	ALA	6.7
36	BO	69	ASP	6.7
26	DD	90	PHE	6.7
17	CR	19	GLU	6.6
48	D1	11	VAL	6.6
48	D1	10	LEU	6.6
50	B3	39	ARG	6.6
40	BS	89	ALA	6.6
40	BS	93	ALA	6.6
36	BO	53	THR	6.6
34	BM	2	LEU	6.6
33	DL	47	ARG	6.6
51	D4	25	VAL	6.6
27	DE	198	GLU	6.6
51	D4	30	GLU	6.6
33	BL	71	ALA	6.5
34	BM	55	ARG	6.5
49	B2	15	SER	6.5
32	DK	120	PRO	6.5
42	BU	90	LYS	6.5
31	BJ	44	TYR	6.5
43	BW	79	ILE	6.5
30	BH	28	ASN	6.5
39	DR	78	ARG	6.5
31	BJ	46	PRO	6.5
27	BE	74	LYS	6.5
33	BL	28	GLY	6.5
42	BU	91	LYS	6.5
26	BD	14	ILE	6.5
51	D4	20	ASP	6.5
25	DC	256	THR	6.5
27	BE	200	LEU	6.5
38	DQ	116	LEU	6.5
42	BU	14	THR	6.5
52	BI	53	PRO	6.5
26	BD	34	VAL	6.5
27	DE	169	VAL	6.5
1	CA	1362	A	6.5
25	DC	59	GLN	6.5
33	DL	58	TYR	6.5
33	DL	53	GLY	6.5
43	DW	35	ILE	6.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
10	CK	125	LYS	6.4
39	BR	41	ILE	6.4
27	DE	172	ALA	6.4
25	BC	43	ASN	6.4
46	BZ	33	ASN	6.4
34	DM	26	VAL	6.4
11	CL	24	GLU	6.4
35	BN	6	SER	6.4
33	DL	92	LEU	6.4
39	DR	82	HIS	6.4
1	AA	121	U	6.4
25	DC	246	PRO	6.4
34	BM	135	VAL	6.4
33	BL	73	ILE	6.4
43	DW	29	SER	6.4
42	DU	28	LEU	6.4
33	BL	62	PRO	6.4
43	DW	6	GLY	6.4
50	B3	43	LEU	6.3
25	DC	156	SER	6.3
47	B0	4	GLN	6.3
36	DO	6	ALA	6.3
42	DU	1	ALA	6.3
43	DW	1	ALA	6.3
47	D0	44	ALA	6.3
33	DL	45	GLY	6.3
33	DL	57	LEU	6.3
50	D3	43	LEU	6.3
38	BQ	35	PHE	6.3
46	DZ	27	THR	6.3
1	AA	78	A	6.3
43	DW	11	ASN	6.3
49	B2	13	ASN	6.3
18	CS	79	TYR	6.3
44	DX	36	GLN	6.3
31	BJ	85	LYS	6.3
45	DY	1	ALA	6.2
25	DC	258	SER	6.2
27	BE	107	SER	6.2
33	BL	26	GLY	6.2
38	BQ	3	VAL	6.2
50	D3	36	ALA	6.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
24	DV	12	GLN	6.2
25	BC	178	GLY	6.2
34	BM	103	TYR	6.2
31	BJ	99	ARG	6.2
8	AI	128	LYS	6.2
11	AL	43	LYS	6.2
42	BU	38	ILE	6.2
46	BZ	19	GLY	6.1
25	BC	51	ARG	6.1
51	D4	4	ARG	6.1
35	BN	69	ARG	6.1
27	BE	188	MET	6.1
35	DN	1	MET	6.1
42	DU	69	VAL	6.1
33	BL	12	SER	6.1
23	DB	2134	A	6.1
26	BD	156	PHE	6.1
23	BB	2104	C	6.1
25	DC	160	TYR	6.1
37	DP	60	VAL	6.1
51	D4	5	ALA	6.1
36	BO	9	ARG	6.1
26	BD	137	SER	6.1
25	DC	238	ASN	6.1
46	DZ	13	THR	6.1
33	BL	50	PHE	6.1
38	DQ	31	TYR	6.1
42	DU	61	GLU	6.0
44	DX	40	SER	6.0
38	DQ	88	GLU	6.0
51	B4	10	LEU	6.0
25	BC	154	ALA	6.0
43	DW	39	GLN	6.0
47	D0	3	GLN	6.0
33	DL	50	PHE	6.0
43	BW	53	GLY	6.0
41	DT	57	VAL	6.0
21	CU	37	TYR	6.0
42	DU	67	SER	6.0
27	DE	27	LEU	6.0
38	DQ	87	VAL	6.0
50	D3	1	PRO	6.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
39	DR	92	TRP	6.0
19	CT	67	HIS	6.0
35	BN	71	ARG	5.9
38	BQ	32	ARG	5.9
44	DX	37	LEU	5.9
46	DZ	31	ASP	5.9
26	DD	79	LEU	5.9
31	DJ	1	MET	5.9
38	DQ	32	ARG	5.9
5	CF	96	VAL	5.9
33	DL	62	PRO	5.9
34	BM	98	PRO	5.9
42	BU	87	GLU	5.9
50	B3	44	ARG	5.9
31	DJ	84	ILE	5.9
9	CJ	47	GLU	5.9
31	DJ	89	PHE	5.9
43	DW	73	PRO	5.9
42	DU	25	LYS	5.9
34	DM	135	VAL	5.9
35	BN	2	ARG	5.8
46	DZ	11	GLU	5.8
52	BI	27	LEU	5.8
23	BB	2154	A	5.8
25	BC	21	PRO	5.8
16	AQ	5	ARG	5.8
26	BD	46	ARG	5.8
38	BQ	47	ARG	5.8
26	DD	140	HIS	5.8
26	DD	101	PHE	5.8
31	DJ	10	THR	5.8
26	BD	138	LEU	5.8
33	BL	64	PHE	5.8
26	BD	61	THR	5.8
43	BW	70	VAL	5.8
33	DL	11	GLY	5.8
33	BL	23	ILE	5.8
29	DG	2	ARG	5.8
25	BC	29	PHE	5.8
43	DW	44	PHE	5.7
50	B3	42	HIS	5.7
39	DR	85	LYS	5.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	BL	98	ALA	5.7
27	BE	164	LEU	5.7
43	BW	58	LEU	5.7
26	BD	131	ASP	5.7
36	BO	76	LYS	5.7
42	DU	3	LYS	5.7
34	DM	132	THR	5.7
27	DE	36	ALA	5.7
35	BN	126	ALA	5.7
49	B2	5	PHE	5.7
25	DC	164	VAL	5.7
40	BS	92	ARG	5.7
25	DC	57	HIS	5.7
1	AA	1362	A	5.7
44	DX	24	GLU	5.7
39	BR	39	LEU	5.7
51	D4	3	VAL	5.7
46	DZ	49	ARG	5.7
27	DE	37	ALA	5.6
3	AD	205	LYS	5.6
36	DO	1	MET	5.6
34	BM	22	GLN	5.6
33	BL	24	GLY	5.6
34	BM	83	GLY	5.6
46	DZ	6	HIS	5.6
26	DD	91	THR	5.6
39	BR	45	GLU	5.6
39	BR	24	LYS	5.6
36	DO	30	ARG	5.6
39	DR	98	ILE	5.6
48	D1	16	THR	5.6
27	BE	199	MET	5.6
27	DE	170	ARG	5.6
46	DZ	41	HIS	5.6
37	DP	75	THR	5.6
46	BZ	11	GLU	5.6
29	DG	3	VAL	5.6
40	BS	9	HIS	5.6
11	CL	22	ALA	5.6
39	DR	26	ASP	5.5
26	DD	125	TRP	5.5
25	BC	156	SER	5.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
41	BT	27	SER	5.5
43	DW	4	LYS	5.5
38	DQ	19	GLN	5.5
50	D3	30	HIS	5.5
35	BN	1	MET	5.5
35	BN	7	GLY	5.5
34	DM	18	ARG	5.5
39	BR	92	TRP	5.5
38	DQ	117	ALA	5.5
27	BE	85	PHE	5.5
50	B3	60	CYS	5.5
24	DV	14	LYS	5.5
40	DS	95	ARG	5.5
23	DB	141	G	5.5
41	BT	79	ASP	5.5
27	DE	87	ALA	5.5
31	DJ	4	PHE	5.5
42	DU	76	THR	5.5
34	BM	18	ARG	5.5
43	DW	19	ARG	5.5
25	BC	40	GLY	5.5
25	BC	30	ALA	5.5
31	DJ	124	VAL	5.5
45	BY	17	PRO	5.4
35	BN	64	ARG	5.4
38	BQ	91	ARG	5.4
27	BE	158	PHE	5.4
39	BR	55	ASP	5.4
35	BN	65	LEU	5.4
41	BT	25	GLU	5.4
26	DD	151	THR	5.4
44	DX	34	SER	5.4
37	BP	96	LEU	5.4
25	DC	51	ARG	5.4
26	BD	89	GLU	5.4
7	CH	7	ALA	5.4
26	DD	204	LYS	5.4
31	BJ	73	VAL	5.4
50	B3	1	PRO	5.4
29	BG	59	ASP	5.4
36	BO	6	ALA	5.4
27	DE	196	VAL	5.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
27	BE	143	LEU	5.4
38	BQ	50	ARG	5.4
1	AA	86	G	5.4
24	DV	13	GLY	5.4
25	DC	210	ALA	5.4
33	BL	117	THR	5.4
50	D3	62	PRO	5.3
45	BY	19	HIS	5.3
47	D0	33	SER	5.3
9	AJ	59	LYS	5.3
13	CN	72	PHE	5.3
36	DO	99	TYR	5.3
43	DW	30	VAL	5.3
46	BZ	9	TYR	5.3
35	DN	3	HIS	5.3
46	DZ	20	ASN	5.3
31	BJ	100	VAL	5.3
26	BD	35	THR	5.3
45	DY	3	THR	5.3
43	BW	3	LYS	5.3
47	B0	3	GLN	5.3
20	AB	212	TYR	5.3
26	BD	125	TRP	5.3
25	DC	47	ARG	5.3
27	DE	42	GLY	5.3
37	BP	50	ARG	5.3
27	DE	200	LEU	5.3
42	DU	68	ASN	5.3
31	BJ	81	ILE	5.3
42	BU	88	ASP	5.3
25	DC	49	THR	5.3
33	DL	74	THR	5.3
22	DA	88	C	5.3
25	BC	258	SER	5.2
33	BL	93	ASN	5.2
23	BB	139	U	5.2
25	BC	256	THR	5.2
31	BJ	7	LYS	5.2
25	DC	3	VAL	5.2
33	DL	20	GLY	5.2
51	B4	25	VAL	5.2
35	BN	66	ALA	5.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
38	DQ	86	SER	5.2
8	CI	128	LYS	5.2
26	BD	99	GLU	5.2
36	DO	24	THR	5.2
26	DD	152	PRO	5.2
43	BW	73	PRO	5.2
25	BC	250	GLN	5.2
28	DF	24	VAL	5.2
27	BE	160	ALA	5.2
39	BR	28	ALA	5.2
49	D2	22	MET	5.2
47	B0	27	LEU	5.2
37	DP	32	VAL	5.2
25	BC	149	LYS	5.2
38	DQ	40	LYS	5.2
39	BR	101	ILE	5.2
25	BC	177	SER	5.2
33	BL	48	ARG	5.2
27	DE	173	THR	5.2
35	BN	70	THR	5.2
27	DE	153	LEU	5.2
25	DC	208	GLY	5.2
45	BY	49	ALA	5.2
45	DY	2	LYS	5.2
31	BJ	84	ILE	5.2
21	CU	34	ARG	5.2
51	B4	36	ARG	5.2
33	DL	42	SER	5.2
48	D1	13	SER	5.2
43	BW	9	THR	5.2
47	B0	38	LEU	5.2
17	AR	39	VAL	5.2
34	BM	93	VAL	5.2
26	DD	132	ALA	5.1
33	BL	65	GLY	5.1
34	BM	68	PHE	5.1
42	DU	7	ASP	5.1
33	BL	47	ARG	5.1
23	DB	2157	G	5.1
27	BE	60	TRP	5.1
27	BE	72	SER	5.1
29	DG	167	VAL	5.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
36	DO	65	THR	5.1
25	DC	43	ASN	5.1
50	D3	27	ASN	5.1
37	BP	3	ILE	5.1
37	BP	4	ILE	5.1
37	BP	109	ILE	5.1
31	DJ	135	GLN	5.1
25	DC	19	VAL	5.1
27	DE	2	GLU	5.1
34	BM	31	PHE	5.1
25	BC	48	ILE	5.1
33	DL	33	ARG	5.1
36	BO	7	ARG	5.1
36	DO	61	GLN	5.1
50	D3	63	TYR	5.1
25	DC	235	GLU	5.1
35	BN	127	GLU	5.1
33	DL	64	PHE	5.1
46	BZ	24	ILE	5.1
43	DW	2	HIS	5.1
27	BE	163	ASN	5.1
23	DB	62	U	5.1
42	DU	60	LYS	5.1
46	DZ	47	LYS	5.1
25	DC	224	MET	5.1
25	DC	64	VAL	5.1
26	DD	68	PHE	5.0
17	AR	20	ILE	5.0
16	AQ	69	THR	5.0
26	BD	167	ASN	5.0
43	DW	52	CYS	5.0
27	DE	201	ALA	5.0
50	D3	31	ILE	5.0
31	BJ	9	GLU	5.0
37	DP	24	THR	5.0
37	DP	103	THR	5.0
46	DZ	2	LYS	5.0
39	BR	1	MET	5.0
33	DL	107	PHE	5.0
41	DT	37	ASP	5.0
28	DF	74	ALA	5.0
34	BM	56	ALA	5.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
27	DE	25	GLU	5.0
31	DJ	15	TRP	5.0
26	BD	92	VAL	5.0
33	DL	46	VAL	5.0
38	BQ	7	VAL	5.0
41	BT	67	VAL	5.0
35	BN	9	GLN	5.0
45	DY	29	ARG	5.0
46	BZ	20	ASN	5.0
50	D3	7	ARG	5.0
23	DB	1	G	5.0
33	BL	103	ILE	5.0
37	DP	68	GLY	5.0
39	BR	56	GLY	5.0
27	BE	144	GLU	5.0
25	DC	257	ARG	5.0
25	DC	268	ARG	5.0
43	DW	40	ARG	5.0
34	DM	109	PRO	5.0
26	BD	116	LYS	5.0
29	DG	59	ASP	5.0
43	DW	74	LYS	5.0
26	DD	9	VAL	4.9
28	BF	131	VAL	4.9
31	BJ	80	HIS	4.9
33	BL	43	GLY	4.9
34	BM	136	MET	4.9
34	DM	40	ARG	4.9
27	DE	50	ALA	4.9
33	BL	9	ALA	4.9
45	DY	10	ARG	4.9
37	DP	33	GLU	4.9
26	BD	155	VAL	4.9
51	D4	33	HIS	4.9
43	DW	67	LYS	4.9
36	DO	57	ALA	4.9
23	DB	919	U	4.9
34	DM	47	GLU	4.9
35	BN	60	VAL	4.9
39	DR	62	GLU	4.9
39	DR	64	VAL	4.9
1	CA	461	A	4.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
47	D0	43	THR	4.9
16	AQ	44	HIS	4.9
26	DD	134	HIS	4.9
31	BJ	120	ARG	4.9
52	BI	127	SER	4.9
27	DE	199	MET	4.9
23	BB	2153	C	4.9
25	DC	151	GLY	4.9
35	DN	2	ARG	4.9
27	DE	55	SER	4.9
34	BM	57	VAL	4.8
27	BE	48	THR	4.8
43	DW	79	ILE	4.8
29	DG	39	ALA	4.8
47	D0	55	ALA	4.8
18	CS	2	ARG	4.8
26	DD	13	ARG	4.8
43	DW	7	GLY	4.8
30	DH	21	VAL	4.8
4	AE	21	SER	4.8
5	CF	100	SER	4.8
18	AS	79	TYR	4.8
33	DL	40	SER	4.8
35	BN	119	SER	4.8
26	DD	136	ASN	4.8
39	DR	39	LEU	4.8
45	BY	24	LEU	4.8
38	DQ	91	ARG	4.8
49	B2	41	ARG	4.8
26	BD	164	GLN	4.8
44	BX	44	LYS	4.8
25	DC	136	VAL	4.8
33	DL	4	ASN	4.8
23	DB	1460	U	4.8
29	BG	3	VAL	4.8
18	AS	2	ARG	4.8
27	DE	147	LEU	4.8
52	BI	78	LEU	4.8
27	BE	17	THR	4.8
33	DL	67	THR	4.8
47	D0	37	HIS	4.8
50	B3	30	HIS	4.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	CH	122	GLY	4.8
1	AA	1286	U	4.8
33	DL	19	LEU	4.8
46	BZ	32	LEU	4.8
26	BD	17	GLU	4.8
26	BD	145	SER	4.8
37	DP	26	GLU	4.8
25	BC	238	ASN	4.8
36	DO	29	HIS	4.8
36	BO	49	VAL	4.7
25	DC	269	ARG	4.7
39	BR	93	PHE	4.7
33	BL	70	LYS	4.7
43	BW	8	SER	4.7
25	DC	127	ASN	4.7
47	B0	2	VAL	4.7
46	BZ	4	ASP	4.7
26	DD	128	ARG	4.7
39	DR	84	ARG	4.7
8	CI	126	PHE	4.7
44	DX	42	LEU	4.7
51	D4	10	LEU	4.7
23	DB	101	A	4.7
26	BD	123	LYS	4.7
25	BC	226	PRO	4.7
27	BE	59	PRO	4.7
33	DL	136	GLU	4.7
26	BD	91	THR	4.7
43	BW	15	SER	4.7
47	B0	28	SER	4.7
51	B4	4	ARG	4.7
28	DF	80	GLN	4.7
33	DL	17	LYS	4.7
51	B4	9	LYS	4.7
22	DA	52	A	4.7
35	BN	105	GLY	4.7
51	B4	6	SER	4.7
23	BB	919	U	4.7
25	BC	211	ARG	4.7
47	B0	9	ARG	4.7
25	BC	53	ILE	4.7
36	DO	35	ILE	4.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
37	DP	73	PHE	4.7
49	D2	18	PHE	4.7
35	DN	9	GLN	4.7
25	BC	244	VAL	4.7
26	DD	166	GLY	4.7
29	DG	172	GLU	4.7
16	CQ	5	ARG	4.7
23	DB	898	C	4.7
38	DQ	50	ARG	4.7
49	D2	43	THR	4.7
27	BE	105	LEU	4.7
52	BI	58	ILE	4.7
11	CL	85	ARG	4.6
29	BG	42	VAL	4.6
33	BL	49	GLY	4.6
37	DP	47	ILE	4.6
40	DS	3	THR	4.6
42	BU	3	LYS	4.6
42	DU	99	SER	4.6
23	BB	2146	C	4.6
39	DR	11	GLN	4.6
41	BT	80	TRP	4.6
42	DU	88	ASP	4.6
32	DK	15	GLY	4.6
33	DL	85	VAL	4.6
49	B2	28	ARG	4.6
49	D2	19	ARG	4.6
25	BC	246	PRO	4.6
5	CF	94	HIS	4.6
27	BE	3	LEU	4.6
31	DJ	76	HIS	4.6
3	AD	19	PHE	4.6
25	BC	37	SER	4.6
36	BO	5	SER	4.6
27	DE	86	ALA	4.6
49	D2	26	ASN	4.6
37	BP	74	GLN	4.6
27	BE	141	MET	4.6
39	DR	80	ARG	4.6
23	BB	1175	A	4.6
27	BE	71	GLY	4.6
10	AK	125	LYS	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
37	DP	96	LEU	4.6
51	D4	15	LYS	4.6
33	BL	22	GLY	4.6
33	BL	29	LYS	4.6
44	DX	35	GLY	4.6
45	BY	41	PRO	4.6
50	D3	38	LYS	4.6
46	DZ	60	PHE	4.6
30	DH	111	ALA	4.6
45	DY	11	SER	4.6
30	DH	33	GLN	4.6
33	DL	38	GLN	4.6
25	DC	212	TRP	4.6
27	BE	54	GLY	4.6
45	BY	23	LEU	4.6
27	BE	129	PRO	4.6
26	BD	64	GLU	4.6
39	BR	16	GLU	4.6
39	BR	23	GLU	4.6
25	BC	251	THR	4.6
34	DM	71	LYS	4.5
34	BM	32	GLY	4.5
25	BC	7	PRO	4.5
18	CS	36	ARG	4.5
33	BL	33	ARG	4.5
33	BL	78	ARG	4.5
15	AP	81	ALA	4.5
31	BJ	63	ALA	4.5
34	DM	134	THR	4.5
35	BN	68	ALA	4.5
34	BM	1	MET	4.5
25	DC	153	LEU	4.5
23	DB	278	A	4.5
38	DQ	51	GLN	4.5
1	AA	765	G	4.5
28	BF	64	PRO	4.5
31	DJ	110	PRO	4.5
33	BL	8	PRO	4.5
25	BC	199	HIS	4.5
27	BE	88	ARG	4.5
31	DJ	88	THR	4.5
21	CU	28	LEU	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
36	DO	62	LEU	4.5
27	DE	38	GLY	4.5
16	CQ	4	ILE	4.5
39	BR	98	ILE	4.5
39	DR	74	ILE	4.5
25	BC	28	PRO	4.5
36	BO	92	PHE	4.5
40	DS	108	SER	4.5
46	BZ	17	SER	4.5
23	BB	1275	A	4.5
43	DW	9	THR	4.5
29	DG	142	GLN	4.5
44	BX	45	GLN	4.5
26	BD	101	PHE	4.5
39	BR	77	PHE	4.5
41	BT	77	ARG	4.5
33	BL	27	LEU	4.5
33	DL	28	GLY	4.5
23	BB	1538	G	4.5
25	BC	47	ARG	4.5
35	DN	4	ARG	4.5
52	BI	79	LEU	4.4
39	BR	79	ARG	4.4
27	BE	177	PRO	4.4
41	DT	80	TRP	4.4
34	BM	97	GLN	4.4
42	DU	45	GLN	4.4
46	DZ	3	LYS	4.4
20	CB	198	VAL	4.4
23	BB	1537	G	4.4
34	DM	2	LEU	4.4
43	BW	2	HIS	4.4
38	DQ	39	ILE	4.4
40	BS	104	THR	4.4
41	DT	74	ILE	4.4
35	BN	72	ASP	4.4
50	D3	53	ASP	4.4
41	BT	26	LYS	4.4
46	BZ	48	GLN	4.4
21	AU	37	TYR	4.4
12	AM	88	LEU	4.4
46	BZ	10	GLU	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
18	AS	76	THR	4.4
37	DP	28	LYS	4.4
44	DX	44	LYS	4.4
25	BC	212	TRP	4.4
25	DC	60	ALA	4.4
31	DJ	118	MET	4.4
52	BI	6	ALA	4.4
44	BX	46	VAL	4.4
31	BJ	121	LYS	4.4
37	DP	22	GLY	4.4
43	BW	77	LYS	4.4
46	DZ	23	LYS	4.4
47	D0	56	LYS	4.4
39	BR	29	THR	4.4
3	CD	49	ASP	4.4
33	DL	27	LEU	4.4
50	B3	48	MET	4.4
25	BC	219	VAL	4.4
38	DQ	38	VAL	4.4
3	AD	197	HIS	4.4
33	BL	135	ILE	4.4
37	DP	56	SER	4.4
25	BC	235	GLU	4.4
52	DI	117	THR	4.4
27	BE	5	LEU	4.3
7	CH	129	ALA	4.3
32	BK	122	VAL	4.3
42	DU	41	VAL	4.3
41	DT	73	ARG	4.3
27	BE	194	LYS	4.3
33	DL	14	LYS	4.3
30	DH	24	GLY	4.3
31	BJ	119	PHE	4.3
42	BU	37	GLY	4.3
23	DB	1175	A	4.3
10	AK	128	VAL	4.3
25	DC	154	ALA	4.3
27	DE	146	VAL	4.3
52	DI	138	VAL	4.3
19	AT	12	GLN	4.3
28	DF	132	ARG	4.3
29	BG	57	TYR	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
52	DI	91	LYS	4.3
26	BD	144	GLY	4.3
34	BM	117	PHE	4.3
27	BE	70	SER	4.3
44	DX	28	LEU	4.3
27	BE	69	ARG	4.3
31	DJ	18	VAL	4.3
42	DU	6	ARG	4.3
1	CA	266	G	4.3
23	DB	2156	G	4.3
50	D3	46	LYS	4.3
22	BA	88	C	4.3
36	DO	97	PHE	4.3
26	DD	183	GLU	4.3
42	DU	32	LYS	4.3
49	D2	37	LYS	4.3
26	DD	14	ILE	4.3
33	DL	54	GLN	4.3
36	BO	19	GLN	4.3
45	BY	52	PHE	4.3
52	DI	136	GLY	4.3
21	CU	10	PRO	4.3
8	CI	15	ALA	4.3
26	BD	151	THR	4.3
26	BD	160	LYS	4.3
28	DF	148	VAL	4.3
8	CI	65	THR	4.3
43	BW	46	ALA	4.3
50	B3	24	LYS	4.3
25	BC	225	ASN	4.3
40	BS	40	ASN	4.3
42	BU	71	ILE	4.3
12	AM	85	TYR	4.3
25	BC	57	HIS	4.3
27	DE	92	HIS	4.3
46	BZ	50	ASP	4.3
23	BB	1509	A	4.2
34	DM	101	VAL	4.2
7	AH	1	SER	4.2
23	BB	137	U	4.2
8	AI	34	LEU	4.2
28	DF	151	LEU	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
51	B4	38	GLY	4.2
33	BL	69	ARG	4.2
46	DZ	58	ASP	4.2
47	B0	49	ARG	4.2
28	DF	68	LYS	4.2
43	BW	4	LYS	4.2
25	BC	267	VAL	4.2
34	BM	69	PRO	4.2
37	BP	24	THR	4.2
51	D4	26	ILE	4.2
19	AT	2	ASN	4.2
49	D2	13	ASN	4.2
38	DQ	58	GLN	4.2
30	BH	122	LEU	4.2
23	BB	1738	G	4.2
27	BE	114	ARG	4.2
31	DJ	82	GLY	4.2
33	DL	18	ARG	4.2
36	DO	2	ASP	4.2
21	AU	35	GLU	4.2
27	BE	2	GLU	4.2
51	B4	28	SER	4.2
33	DL	69	ARG	4.2
6	AG	113	LYS	4.2
29	BG	176	LYS	4.2
11	AL	71	HIS	4.2
37	BP	79	VAL	4.2
36	BO	12	THR	4.2
33	DL	3	LEU	4.2
38	DQ	105	PHE	4.2
41	DT	76	ARG	4.2
42	DU	5	ARG	4.2
7	AH	55	LYS	4.2
29	BG	63	GLN	4.2
39	BR	83	TYR	4.2
6	CG	152	HIS	4.2
28	DF	73	VAL	4.2
1	CA	977	A	4.2
40	DS	10	ALA	4.2
36	DO	58	ILE	4.2
25	BC	22	GLU	4.2
46	DZ	10	GLU	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
8	CI	42	THR	4.2
9	AJ	16	ARG	4.2
14	AO	88	ARG	4.2
25	DC	172	THR	4.2
31	BJ	37	ARG	4.2
46	DZ	59	ARG	4.2
25	BC	27	LYS	4.2
26	BD	90	PHE	4.2
51	D4	32	LYS	4.2
34	DM	83	GLY	4.1
7	AH	2	MET	4.1
52	BI	11	GLN	4.1
36	DO	34	HIS	4.1
6	AG	4	ARG	4.1
3	AD	150	LYS	4.1
11	AL	9	LYS	4.1
27	DE	132	LYS	4.1
27	DE	140	ASP	4.1
23	DB	139	U	4.1
30	BH	93	SER	4.1
39	DR	33	VAL	4.1
51	D4	29	ALA	4.1
16	CQ	3	LYS	4.1
27	DE	138	LEU	4.1
52	BI	10	LEU	4.1
29	DG	51	PHE	4.1
34	BM	134	THR	4.1
1	AA	1441	A	4.1
23	DB	2135	A	4.1
7	CH	127	TYR	4.1
44	DX	39	GLN	4.1
3	AD	36	ALA	4.1
17	AR	73	HIS	4.1
34	DM	56	ALA	4.1
36	BO	70	ALA	4.1
38	DQ	45	ALA	4.1
25	BC	127	ASN	4.1
26	DD	146	ILE	4.1
37	BP	49	ILE	4.1
31	DJ	120	ARG	4.1
11	CL	75	GLU	4.1
33	BL	136	GLU	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
39	BR	37	GLU	4.1
26	DD	129	THR	4.1
28	BF	152	ASP	4.1
41	BT	37	ASP	4.1
46	BZ	13	THR	4.1
11	AL	117	GLY	4.1
39	BR	51	VAL	4.1
50	D3	6	VAL	4.1
6	AG	8	GLN	4.1
25	DC	30	ALA	4.1
27	BE	37	ALA	4.1
13	AN	60	ARG	4.1
18	AS	36	ARG	4.1
23	DB	2799	A	4.1
25	DC	103	ILE	4.1
25	DC	199	HIS	4.1
27	BE	15	SER	4.1
38	DQ	12	ARG	4.1
16	AQ	36	PHE	4.1
13	CN	94	GLY	4.1
25	DC	41	GLY	4.1
34	BM	131	VAL	4.1
34	DM	25	ASP	4.1
3	AD	43	ARG	4.1
32	DK	71	ARG	4.1
51	B4	5	ALA	4.1
51	B4	29	ALA	4.1
39	DR	86	GLN	4.1
10	AK	49	SER	4.1
26	DD	145	SER	4.1
27	BE	80	SER	4.1
26	DD	126	ASN	4.1
8	CI	111	GLU	4.0
28	DF	133	GLU	4.0
34	BM	108	VAL	4.0
1	AA	1214	C	4.0
18	AS	32	THR	4.0
8	CI	123	ARG	4.0
11	AL	8	ARG	4.0
26	DD	59	ARG	4.0
36	BO	3	LYS	4.0
43	BW	67	LYS	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
46	BZ	23	LYS	4.0
50	B3	64	ALA	4.0
52	BI	1	ALA	4.0
52	BI	13	ALA	4.0
52	DI	2	LYS	4.0
17	CR	63	TYR	4.0
33	DL	101	ILE	4.0
43	BW	35	ILE	4.0
18	AS	9	PHE	4.0
42	DU	95	PHE	4.0
40	BS	1	MET	4.0
52	BI	124	MET	4.0
23	DB	1236	G	4.0
33	BL	122	VAL	4.0
37	DP	104	GLY	4.0
42	DU	56	GLY	4.0
8	AI	123	ARG	4.0
33	BL	36	LYS	4.0
36	DO	3	LYS	4.0
49	D2	28	ARG	4.0
29	DG	46	ASP	4.0
38	BQ	96	ASP	4.0
23	DB	645	C	4.0
31	DJ	86	GLN	4.0
44	DX	1	MET	4.0
26	BD	9	VAL	4.0
40	DS	107	VAL	4.0
42	BU	82	VAL	4.0
43	BW	50	VAL	4.0
15	CP	28	ARG	4.0
27	DE	79	ARG	4.0
27	DE	111	GLU	4.0
30	BH	92	GLY	4.0
35	DN	123	GLU	4.0
38	DQ	92	LYS	4.0
4	AE	89	THR	4.0
5	AF	51	ILE	4.0
26	DD	197	THR	4.0
31	BJ	133	ALA	4.0
50	B3	58	ILE	4.0
51	D4	14	CYS	4.0
51	B4	20	ASP	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	CD	114	ARG	4.0
19	CT	63	LYS	4.0
25	BC	257	ARG	4.0
39	BR	84	ARG	4.0
52	DI	133	ARG	4.0
33	BL	32	GLY	4.0
37	DP	43	GLU	4.0
18	AS	30	LEU	4.0
20	CB	165	ALA	4.0
33	BL	97	ALA	4.0
5	CF	92	THR	4.0
37	BP	98	TYR	4.0
37	DP	19	PHE	4.0
39	DR	6	GLN	4.0
21	CU	53	LYS	4.0
34	BM	5	LYS	4.0
23	DB	1459	G	4.0
47	D0	53	VAL	4.0
42	BU	31	GLY	4.0
49	B2	8	SER	4.0
11	CL	1	ALA	4.0
35	BN	123	GLU	4.0
8	AI	42	THR	4.0
26	BD	143	PRO	4.0
36	DO	92	PHE	3.9
26	DD	94	GLN	3.9
9	CJ	59	LYS	3.9
26	BD	128	ARG	3.9
37	BP	95	LYS	3.9
37	DP	92	ARG	3.9
38	BQ	49	ARG	3.9
40	DS	73	LYS	3.9
27	BE	120	VAL	3.9
23	DB	2833	U	3.9
26	DD	96	ILE	3.9
37	DP	65	ASN	3.9
12	CM	101	THR	3.9
26	DD	154	LYS	3.9
27	DE	74	LYS	3.9
28	DF	70	ARG	3.9
34	BM	16	ARG	3.9
52	DI	97	VAL	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
46	BZ	5	ILE	3.9
52	BI	85	ILE	3.9
33	BL	15	ALA	3.9
18	CS	3	SER	3.9
37	BP	56	SER	3.9
23	BB	1847	A	3.9
41	BT	28	ASN	3.9
4	CE	158	LYS	3.9
27	BE	19	PHE	3.9
42	DU	23	LYS	3.9
46	DZ	43	PHE	3.9
13	CN	58	ARG	3.9
36	DO	10	ARG	3.9
23	BB	1087	G	3.9
23	DB	2110	G	3.9
26	BD	146	ILE	3.9
30	BH	12	LEU	3.9
2	AC	136	ALA	3.9
35	DN	5	LYS	3.9
36	BO	45	SER	3.9
51	D4	28	SER	3.9
34	DM	50	ARG	3.9
35	DN	8	ARG	3.9
48	B1	38	PHE	3.9
13	AN	66	THR	3.9
26	BD	11	MET	3.9
27	DE	1	MET	3.9
52	DI	7	TYR	3.9
26	BD	198	GLY	3.9
30	DH	72	ILE	3.9
26	DD	71	ALA	3.9
43	BW	14	ASP	3.9
50	D3	4	LYS	3.9
52	BI	9	LYS	3.9
50	B3	41	ARG	3.9
8	AI	127	SER	3.9
13	AN	51	PRO	3.9
26	BD	113	SER	3.9
48	D1	12	SER	3.9
2	AC	18	ASN	3.9
34	BM	101	VAL	3.9
39	BR	82	HIS	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
25	DC	173	LEU	3.9
25	DC	48	ILE	3.9
27	BE	136	GLN	3.9
33	BL	3	LEU	3.9
39	BR	11	GLN	3.9
23	DB	1057	A	3.9
18	AS	11	ASP	3.9
25	DC	35	LYS	3.9
39	DR	73	LYS	3.9
47	B0	51	ARG	3.9
27	DE	19	PHE	3.8
52	BI	135	MET	3.8
8	CI	8	THR	3.8
42	BU	69	VAL	3.8
18	AS	13	HIS	3.8
23	BB	2148	G	3.8
30	BH	143	ILE	3.8
23	BB	932	U	3.8
6	AG	116	ALA	3.8
20	AB	74	ALA	3.8
35	DN	91	ALA	3.8
38	DQ	4	LYS	3.8
39	BR	3	ALA	3.8
51	D4	18	LYS	3.8
52	BI	2	LYS	3.8
25	DC	42	ARG	3.8
1	CA	1441	A	3.8
41	DT	63	VAL	3.8
9	AJ	83	THR	3.8
42	DU	102	ILE	3.8
27	BE	38	GLY	3.8
29	BG	68	ARG	3.8
36	BO	16	ARG	3.8
39	DR	90	ARG	3.8
27	DE	168	ASP	3.8
31	DJ	91	GLU	3.8
52	BI	69	VAL	3.8
1	AA	51	A	3.8
23	BB	63	A	3.8
33	DL	61	LEU	3.8
51	D4	16	ILE	3.8
31	DJ	80	HIS	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
27	DE	24	ASN	3.8
33	DL	49	GLY	3.8
37	DP	61	ARG	3.8
42	BU	56	GLY	3.8
25	BC	60	ALA	3.8
27	DE	190	ALA	3.8
25	DC	21	PRO	3.8
26	BD	98	VAL	3.8
42	BU	24	VAL	3.8
52	DI	23	VAL	3.8
11	CL	103	CYS	3.8
39	DR	45	GLU	3.8
44	DX	21	LEU	3.8
50	B3	3	ILE	3.8
29	BG	2	ARG	3.8
5	CF	95	ALA	3.8
15	CP	43	ALA	3.8
31	DJ	51	GLY	3.8
38	BQ	98	ALA	3.8
15	AP	29	ASN	3.8
34	BM	17	ASN	3.8
26	DD	164	GLN	3.8
37	DP	74	GLN	3.8
42	DU	65	GLN	3.8
20	AB	24	PRO	3.8
34	DM	108	VAL	3.8
49	D2	10	LEU	3.8
1	AA	1302	C	3.8
33	DL	51	GLU	3.8
25	BC	266	ILE	3.8
42	BU	25	LYS	3.8
47	B0	42	ILE	3.8
20	AB	94	ARG	3.8
12	AM	107	THR	3.8
25	BC	222	THR	3.8
9	CJ	12	ALA	3.8
25	BC	126	GLY	3.8
31	DJ	107	GLY	3.8
45	DY	27	GLY	3.8
49	D2	23	ALA	3.8
25	DC	177	SER	3.7
50	B3	50	SER	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
26	BD	136	ASN	3.7
31	BJ	86	GLN	3.7
40	BS	61	ASN	3.7
42	BU	84	PHE	3.7
26	DD	155	VAL	3.7
46	DZ	21	VAL	3.7
31	DJ	109	LEU	3.7
44	DX	43	LEU	3.7
52	BI	22	PRO	3.7
27	BE	132	LYS	3.7
52	DI	9	LYS	3.7
28	DF	84	ILE	3.7
35	DN	120	GLU	3.7
34	DM	106	ASP	3.7
51	D4	11	CYS	3.7
16	AQ	6	THR	3.7
26	BD	166	GLY	3.7
27	BE	11	ALA	3.7
31	DJ	134	ALA	3.7
33	BL	108	ALA	3.7
39	BR	8	GLY	3.7
52	DI	6	ALA	3.7
23	BB	62	U	3.7
27	BE	165	HIS	3.7
47	B0	41	HIS	3.7
10	AK	60	PHE	3.7
13	CN	54	SER	3.7
33	DL	66	PHE	3.7
35	DN	119	SER	3.7
5	AF	52	ASN	3.7
36	BO	43	ASN	3.7
42	BU	68	ASN	3.7
45	DY	53	MET	3.7
48	B1	25	ASN	3.7
40	DS	46	LEU	3.7
47	D0	21	LEU	3.7
52	DI	4	VAL	3.7
26	DD	80	TRP	3.7
26	DD	205	PRO	3.7
27	BE	78	TRP	3.7
27	DE	47	LYS	3.7
27	DE	60	TRP	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	BL	96	LYS	3.7
46	BZ	47	LYS	3.7
49	D2	41	ARG	3.7
23	BB	1074	G	3.7
23	DB	277	G	3.7
23	DB	1401	G	3.7
21	CU	35	GLU	3.7
35	BN	43	GLU	3.7
12	AM	98	GLY	3.7
20	AB	11	ALA	3.7
25	DC	65	ASP	3.7
26	DD	31	ALA	3.7
27	BE	128	ALA	3.7
34	BM	122	ALA	3.7
34	BM	132	THR	3.7
48	D1	20	TYR	3.7
7	CH	75	GLN	3.7
41	DT	67	VAL	3.7
46	DZ	36	VAL	3.7
34	BM	8	LYS	3.7
52	DI	53	PRO	3.7
40	BS	66	ILE	3.7
15	AP	82	ALA	3.7
31	BJ	112	GLY	3.7
44	DX	63	ALA	3.7
23	DB	654	A	3.7
47	B0	30	ASP	3.7
48	D1	23	THR	3.7
25	DC	204	LEU	3.7
27	DE	109	LEU	3.7
28	DF	39	VAL	3.7
29	DG	5	LYS	3.7
35	BN	98	LEU	3.7
39	BR	64	VAL	3.7
45	BY	55	LYS	3.7
46	DZ	32	LEU	3.7
28	BF	62	GLN	3.7
49	B2	6	GLN	3.7
21	AU	44	ARG	3.7
33	BL	60	ARG	3.7
23	BB	102	U	3.7
12	CM	71	GLU	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
29	DG	45	ALA	3.7
41	DT	71	GLY	3.7
12	CM	62	PHE	3.7
40	DS	82	MET	3.7
43	BW	18	LYS	3.7
46	BZ	6	HIS	3.7
37	DP	15	ASP	3.7
52	BI	4	VAL	3.7
12	CM	89	ARG	3.7
43	DW	10	ARG	3.7
28	DF	134	GLN	3.7
42	DU	53	GLN	3.7
28	DF	110	ILE	3.7
32	BK	38	ILE	3.7
1	CA	765	G	3.7
23	BB	136	G	3.7
23	BB	1210	G	3.7
23	BB	2133	G	3.7
23	DB	1210	G	3.7
6	CG	105	GLU	3.6
8	CI	9	GLY	3.6
34	BM	19	GLY	3.6
43	DW	5	ALA	3.6
13	AN	5	MET	3.6
30	DH	41	LYS	3.6
34	BM	86	LYS	3.6
41	DT	26	LYS	3.6
42	DU	96	LYS	3.6
52	DI	94	LYS	3.6
26	BD	33	ARG	3.6
30	DH	123	ARG	3.6
36	BO	33	ARG	3.6
42	DU	66	VAL	3.6
50	D3	29	ARG	3.6
7	AH	4	ASP	3.6
33	BL	91	ASP	3.6
42	DU	8	ASP	3.6
44	DX	31	GLN	3.6
51	B4	11	CYS	3.6
23	BB	2799	A	3.6
23	DB	2147	A	3.6
36	DO	45	SER	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
25	BC	89	ASN	3.6
6	CG	145	GLU	3.6
27	BE	95	LYS	3.6
46	BZ	44	PHE	3.6
52	BI	116	MET	3.6
11	CL	93	ARG	3.6
21	CU	46	ARG	3.6
38	DQ	7	VAL	3.6
45	DY	37	ARG	3.6
19	AT	67	HIS	3.6
21	CU	41	THR	3.6
39	BR	2	TYR	3.6
11	AL	102	ASP	3.6
20	AB	199	ILE	3.6
26	DD	173	GLN	3.6
28	DF	72	SER	3.6
35	BN	107	ASN	3.6
37	DP	110	LYS	3.6
49	D2	46	LYS	3.6
23	DB	878	A	3.6
6	AG	73	GLU	3.6
26	DD	186	LEU	3.6
40	DS	18	ARG	3.6
48	D1	43	ARG	3.6
52	DI	135	MET	3.6
26	BD	104	VAL	3.6
34	DM	93	VAL	3.6
35	BN	16	HIS	3.6
34	BM	125	PRO	3.6
48	D1	30	PRO	3.6
23	DB	2732	G	3.6
34	DM	127	LYS	3.6
34	DM	133	LYS	3.6
50	D3	34	LYS	3.6
38	BQ	20	ALA	3.6
3	AD	5	GLY	3.6
16	AQ	64	ARG	3.6
31	BJ	69	ARG	3.6
34	DM	82	MET	3.6
36	BO	1	MET	3.6
47	D0	49	ARG	3.6
36	BO	54	VAL	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
26	DD	25	THR	3.6
26	BD	205	PRO	3.6
1	AA	85	U	3.6
1	CA	1224	U	3.6
12	CM	109	LYS	3.6
25	BC	186	ASP	3.6
39	BR	42	ALA	3.6
17	CR	56	ARG	3.6
52	DI	98	GLY	3.6
3	AD	22	SER	3.6
27	DE	80	SER	3.6
23	DB	1071	G	3.6
23	DB	2104	C	3.6
23	DB	2666	C	3.6
27	DE	122	GLU	3.6
32	BK	89	ASN	3.6
31	BJ	75	TYR	3.6
41	DT	70	HIS	3.6
51	B4	26	ILE	3.6
8	CI	119	LYS	3.6
33	DL	109	LYS	3.6
1	AA	532	A	3.5
23	BB	144	A	3.5
23	DB	279	A	3.5
25	DC	211	ARG	3.5
26	DD	69	ALA	3.5
50	D3	59	ALA	3.5
31	BJ	71	ASP	3.5
23	BB	2320	U	3.5
25	DC	112	GLY	3.5
28	DF	85	GLY	3.5
41	BT	24	MET	3.5
46	DZ	22	MET	3.5
25	BC	18	VAL	3.5
25	DC	171	VAL	3.5
26	BD	170	VAL	3.5
33	BL	42	SER	3.5
19	CT	35	TYR	3.5
25	DC	8	THR	3.5
41	BT	29	THR	3.5
52	BI	112	LYS	3.5
36	DO	16	ARG	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
41	BT	76	ARG	3.5
8	AI	51	LEU	3.5
13	CN	45	LEU	3.5
34	BM	3	GLN	3.5
35	DN	124	ALA	3.5
44	DX	33	ALA	3.5
42	DU	94	PHE	3.5
43	BW	59	PHE	3.5
23	DB	1847	A	3.5
30	BH	115	VAL	3.5
30	BH	142	VAL	3.5
42	DU	24	VAL	3.5
46	DZ	50	ASP	3.5
47	D0	30	ASP	3.5
11	AL	24	GLU	3.5
21	CU	7	GLU	3.5
19	AT	68	LYS	3.5
12	AM	101	THR	3.5
17	AR	72	ARG	3.5
30	BH	124	THR	3.5
50	D3	12	ARG	3.5
42	DU	62	ALA	3.5
34	DM	22	GLN	3.5
4	CE	157	GLY	3.5
34	DM	9	PHE	3.5
42	BU	94	PHE	3.5
31	BJ	18	VAL	3.5
46	BZ	21	VAL	3.5
52	BI	8	VAL	3.5
1	AA	266	G	3.5
23	BB	1459	G	3.5
34	BM	11	LYS	3.5
31	DJ	43	GLU	3.5
35	BN	14	SER	3.5
35	DN	59	SER	3.5
40	BS	59	GLU	3.5
22	DA	25	U	3.5
43	DW	45	HIS	3.5
34	BM	24	THR	3.5
49	D2	4	THR	3.5
35	DN	126	ALA	3.5
48	B1	1	ALA	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
52	DI	26	ALA	3.5
44	DX	30	MET	3.5
29	DG	42	VAL	3.5
1	AA	83	C	3.5
27	DE	145	ASP	3.5
39	BR	95	ASP	3.5
42	DU	80	ASP	3.5
3	AD	146	GLU	3.5
6	AG	78	ARG	3.5
25	BC	179	GLU	3.5
36	DO	7	ARG	3.5
36	DO	100	HIS	3.5
25	DC	20	ASN	3.5
28	DF	22	ASN	3.5
50	B3	62	PRO	3.5
32	DK	97	THR	3.5
34	BM	21	ALA	3.5
52	BI	59	THR	3.5
2	CC	1	GLY	3.5
27	DE	158	PHE	3.5
31	BJ	51	GLY	3.5
33	BL	45	GLY	3.5
46	DZ	51	VAL	3.5
52	DI	8	VAL	3.5
44	BX	4	LYS	3.5
27	DE	108	ILE	3.5
38	DQ	93	ILE	3.5
48	D1	47	ILE	3.5
38	BQ	2	ARG	3.5
43	BW	38	ARG	3.5
28	DF	173	ASP	3.5
45	BY	39	ASP	3.5
44	BX	14	LEU	3.4
52	DI	137	LEU	3.4
13	AN	4	SER	3.4
42	DU	47	PRO	3.4
30	DH	64	ALA	3.4
30	DH	106	ALA	3.4
27	BE	131	THR	3.4
27	DE	53	THR	3.4
10	AK	31	VAL	3.4
40	BS	45	VAL	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
15	AP	13	LYS	3.4
1	AA	82	G	3.4
23	BB	2336	A	3.4
33	DL	129	LYS	3.4
40	BS	28	LYS	3.4
23	BB	2645	G	3.4
25	DC	250	GLN	3.4
20	CB	163	ILE	3.4
17	AR	52	ARG	3.4
39	BR	90	ARG	3.4
30	BH	6	LEU	3.4
31	BJ	52	ASP	3.4
33	BL	61	LEU	3.4
35	DN	117	ASP	3.4
49	D2	16	HIS	3.4
13	AN	35	ALA	3.4
13	CN	1	ALA	3.4
30	DH	26	ALA	3.4
36	BO	52	SER	3.4
40	DS	1	MET	3.4
12	AM	62	PHE	3.4
25	DC	190	THR	3.4
26	BD	60	VAL	3.4
30	DH	78	VAL	3.4
30	DH	132	PHE	3.4
36	BO	103	VAL	3.4
45	DY	52	PHE	3.4
52	BI	60	VAL	3.4
9	AJ	38	GLY	3.4
23	BB	143	C	3.4
38	DQ	21	LYS	3.4
41	BT	66	LYS	3.4
13	CN	52	ARG	3.4
48	D1	4	ILE	3.4
50	D3	39	ARG	3.4
23	DB	142	A	3.4
13	AN	50	LEU	3.4
25	BC	153	LEU	3.4
23	BB	2138	G	3.4
2	AC	151	GLU	3.4
25	BC	169	ALA	3.4
25	BC	243	PRO	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
31	BJ	76	HIS	3.4
45	BY	42	ALA	3.4
25	DC	260	LYS	3.4
27	BE	57	LYS	3.4
29	BG	28	LYS	3.4
30	BH	91	PHE	3.4
34	DM	57	VAL	3.4
42	BU	58	VAL	3.4
27	BE	42	GLY	3.4
32	DK	14	SER	3.4
52	BI	87	SER	3.4
12	CM	106	ARG	3.4
20	CB	39	ILE	3.4
38	DQ	73	ILE	3.4
43	DW	36	ILE	3.4
45	BY	30	ARG	3.4
52	BI	128	ILE	3.4
1	CA	632	U	3.4
3	CD	150	LYS	3.4
8	CI	107	ALA	3.4
20	CB	14	HIS	3.4
23	BB	1090	A	3.4
37	BP	26	GLU	3.4
39	DR	40	MET	3.4
25	DC	141	HIS	3.4
42	BU	59	GLU	3.4
46	DZ	30	HIS	3.4
24	BV	56	PHE	3.4
37	DP	42	PHE	3.4
13	AN	67	GLY	3.4
52	DI	84	GLY	3.4
21	CU	33	ARG	3.4
10	CK	25	SER	3.4
25	DC	139	THR	3.4
35	BN	4	ARG	3.4
38	DQ	29	ARG	3.4
27	DE	75	SER	3.4
37	BP	1	SER	3.4
43	BW	57	THR	3.4
45	DY	9	THR	3.4
2	CC	166	TRP	3.4
20	CB	56	LEU	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
31	DJ	2	LYS	3.4
33	DL	141	LYS	3.4
4	CE	83	PRO	3.4
29	DG	53	PRO	3.4
35	BN	109	PRO	3.4
31	BJ	43	GLU	3.4
32	BK	63	VAL	3.4
38	BQ	87	VAL	3.4
38	DQ	110	GLU	3.4
52	BI	138	VAL	3.4
19	AT	23	ARG	3.4
34	DM	32	GLY	3.4
37	DP	112	ARG	3.4
38	DQ	47	ARG	3.4
41	DT	75	GLY	3.4
43	DW	24	ARG	3.4
15	AP	42	ILE	3.4
25	DC	251	THR	3.4
34	BM	65	ILE	3.4
27	BE	138	LEU	3.3
37	DP	54	LEU	3.3
38	DQ	43	GLN	3.3
39	BR	22	LEU	3.3
50	D3	60	CYS	3.3
29	DG	174	LYS	3.3
29	DG	176	LYS	3.3
42	DU	90	LYS	3.3
51	D4	8	LYS	3.3
13	CN	98	ALA	3.3
31	DJ	6	ALA	3.3
31	DJ	62	VAL	3.3
37	DP	48	ALA	3.3
39	DR	54	VAL	3.3
43	BW	22	VAL	3.3
46	BZ	43	PHE	3.3
3	AD	69	ARG	3.3
30	DH	27	ARG	3.3
39	BR	12	HIS	3.3
41	BT	4	GLU	3.3
51	B4	30	GLU	3.3
51	D4	36	ARG	3.3
31	DJ	83	GLY	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
43	DW	26	GLY	3.3
1	AA	372	C	3.3
23	BB	876	C	3.3
25	DC	167	ASP	3.3
27	DE	191	ASP	3.3
28	DF	45	ASP	3.3
16	CQ	6	THR	3.3
26	BD	16	THR	3.3
29	BG	35	THR	3.3
47	D0	25	THR	3.3
5	CF	54	LEU	3.3
28	BF	35	LEU	3.3
44	DX	19	LEU	3.3
52	DI	52	LEU	3.3
30	DH	113	SER	3.3
33	BL	7	SER	3.3
1	AA	1167	A	3.3
28	BF	134	GLN	3.3
26	DD	20	VAL	3.3
29	DG	96	ALA	3.3
30	DH	69	ALA	3.3
35	BN	125	ALA	3.3
52	BI	26	ALA	3.3
3	AD	72	ARG	3.3
28	DF	113	PHE	3.3
34	BM	28	PHE	3.3
37	BP	88	ARG	3.3
39	BR	89	HIS	3.3
7	AH	81	GLY	3.3
29	DG	99	GLY	3.3
33	DL	34	GLY	3.3
41	DT	56	GLU	3.3
48	D1	3	GLY	3.3
1	AA	1039	G	3.3
23	BB	561	G	3.3
16	CQ	83	LEU	3.3
25	BC	172	THR	3.3
25	DC	245	THR	3.3
28	BF	45	ASP	3.3
19	CT	70	LYS	3.3
31	BJ	41	LYS	3.3
36	BO	17	LYS	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
43	BW	23	LYS	3.3
23	BB	1174	U	3.3
8	CI	31	GLN	3.3
30	DH	73	ASN	3.3
17	AR	55	ALA	3.3
52	BI	57	VAL	3.3
1	AA	1492	A	3.3
23	BB	2886	A	3.3
28	BF	83	PRO	3.3
12	AM	83	GLY	3.3
25	DC	179	GLU	3.3
26	DD	88	GLU	3.3
30	DH	149	GLU	3.3
33	BL	76	GLU	3.3
28	DF	13	LYS	3.3
1	CA	251	G	3.3
2	CC	50	SER	3.3
7	AH	117	GLN	3.3
21	CU	16	ARG	3.3
27	BE	49	ARG	3.3
27	BE	94	GLN	3.3
1	CA	121	U	3.3
30	BH	26	ALA	3.3
31	BJ	4	PHE	3.3
36	DO	23	ALA	3.3
36	DO	27	VAL	3.3
41	BT	63	VAL	3.3
48	D1	41	VAL	3.3
52	DI	83	ALA	3.3
28	DF	83	PRO	3.3
33	DL	56	PRO	3.3
36	BO	42	PRO	3.3
21	AU	3	ILE	3.3
25	DC	26	GLY	3.3
50	D3	52	GLY	3.3
23	BB	2147	A	3.3
23	DB	63	A	3.3
26	DD	86	GLU	3.3
36	BO	64	TYR	3.3
47	D0	35	GLU	3.3
52	BI	52	LEU	3.3
5	CF	93	LYS	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
49	D2	25	LYS	3.3
52	DI	81	LYS	3.3
46	BZ	53	THR	3.3
7	CH	2	MET	3.3
9	CJ	60	ASP	3.3
41	DT	79	ASP	3.3
43	BW	54	ARG	3.3
47	D0	45	ASP	3.3
49	D2	33	ARG	3.3
46	DZ	28	VAL	3.3
39	DR	35	PHE	3.3
47	B0	55	ALA	3.3
31	BJ	113	PRO	3.3
28	BF	84	ILE	3.3
38	BQ	93	ILE	3.3
47	B0	46	GLY	3.3
47	D0	34	GLY	3.3
51	B4	18	LYS	3.2
52	DI	80	LYS	3.2
18	CS	64	GLU	3.2
31	DJ	44	TYR	3.2
20	CB	124	THR	3.2
33	BL	126	ARG	3.2
36	BO	10	ARG	3.2
36	BO	15	ARG	3.2
3	AD	200	VAL	3.2
20	CB	220	VAL	3.2
47	B0	53	VAL	3.2
8	AI	19	PHE	3.2
27	DE	23	PHE	3.2
36	BO	117	PHE	3.2
46	DZ	35	ASP	3.2
50	B3	13	PHE	3.2
52	DI	132	ALA	3.2
25	BC	230	PRO	3.2
25	DC	266	ILE	3.2
36	DO	32	PRO	3.2
19	CT	68	LYS	3.2
26	DD	84	LEU	3.2
30	DH	22	LYS	3.2
31	DJ	68	LYS	3.2
43	DW	20	LEU	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
25	BC	52	HIS	3.2
34	DM	13	HIS	3.2
47	B0	37	HIS	3.2
6	CG	128	GLU	3.2
26	DD	74	GLU	3.2
36	DO	94	ARG	3.2
37	DP	30	TRP	3.2
1	CA	481	G	3.2
23	BB	1056	G	3.2
23	DB	1171	G	3.2
23	DB	1738	G	3.2
23	DB	2307	G	3.2
28	BF	145	VAL	3.2
34	BM	89	VAL	3.2
25	DC	29	PHE	3.2
41	BT	38	ALA	3.2
43	DW	48	ALA	3.2
52	BI	68	PHE	3.2
1	AA	1110	A	3.2
7	CH	89	ASP	3.2
23	BB	2134	A	3.2
23	BB	2297	A	3.2
26	DD	131	ASP	3.2
31	BJ	49	ASP	3.2
38	BQ	58	GLN	3.2
2	AC	13	ILE	3.2
19	AT	3	ILE	3.2
19	AT	8	LYS	3.2
21	CU	45	LYS	3.2
33	DL	70	LYS	3.2
52	DI	128	ILE	3.2
48	B1	35	LEU	3.2
52	DI	27	LEU	3.2
4	AE	157	GLY	3.2
3	AD	195	ASN	3.2
15	AP	79	ASN	3.2
40	BS	102	HIS	3.2
19	AT	35	TYR	3.2
35	BN	94	TYR	3.2
39	DR	13	ARG	3.2
44	DX	47	ARG	3.2
1	AA	219	U	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
30	DH	134	VAL	3.2
41	DT	53	VAL	3.2
51	D4	22	VAL	3.2
2	CC	191	THR	3.2
28	BF	106	ALA	3.2
29	BG	164	ALA	3.2
30	DH	65	ALA	3.2
35	BN	21	PHE	3.2
52	BI	70	THR	3.2
52	BI	109	ALA	3.2
52	DI	1	ALA	3.2
31	BJ	135	GLN	3.2
31	DJ	7	LYS	3.2
41	DT	2	ILE	3.2
9	CJ	43	PRO	3.2
36	BO	18	LEU	3.2
36	DO	21	LEU	3.2
24	DV	76	ASP	3.2
49	D2	7	PRO	3.2
4	CE	107	GLY	3.2
33	DL	102	GLY	3.2
43	DW	21	GLY	3.2
1	CA	65	A	3.2
3	CD	48	SER	3.2
10	CK	126	ARG	3.2
20	CB	38	HIS	3.2
25	DC	14	HIS	3.2
48	D1	18	HIS	3.2
45	BY	54	VAL	3.2
21	AU	11	PHE	3.2
30	DH	39	ALA	3.2
43	DW	17	ALA	3.2
37	BP	5	LYS	3.2
37	DP	105	LYS	3.2
38	BQ	92	LYS	3.2
46	DZ	8	LYS	3.2
2	AC	206	ILE	3.2
8	CI	34	LEU	3.2
12	CM	94	LEU	3.2
23	BB	2402	U	3.2
23	BB	2491	U	3.2
23	DB	100	U	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
23	DB	646	U	3.2
25	BC	204	LEU	3.2
28	BF	140	ILE	3.2
31	DJ	101	ILE	3.2
42	DU	4	ILE	3.2
12	CM	111	PRO	3.2
29	BG	21	GLN	3.2
32	BK	71	ARG	3.2
34	BM	70	ASP	3.2
23	BB	982	C	3.2
20	AB	135	MET	3.2
3	CD	66	VAL	3.2
11	AL	118	VAL	3.2
23	BB	1205	A	3.2
23	BB	1808	A	3.2
27	DE	155	GLU	3.2
36	DO	60	GLU	3.2
52	DI	61	TYR	3.2
23	DB	51	G	3.2
13	AN	43	ALA	3.2
19	CT	46	ALA	3.2
26	BD	154	LYS	3.2
29	BG	5	LYS	3.2
40	BS	90	LYS	3.2
8	AI	65	THR	3.2
26	BD	48	ILE	3.2
34	DM	78	LEU	3.2
18	AS	75	PRO	3.1
33	DL	44	GLY	3.1
34	DM	107	GLY	3.1
21	CU	12	ASP	3.1
26	BD	43	ASP	3.1
27	DE	110	SER	3.1
37	DP	77	SER	3.1
5	CF	84	VAL	3.1
34	DM	104	GLU	3.1
37	DP	101	GLU	3.1
1	AA	381	C	3.1
23	BB	2666	C	3.1
25	DC	265	PHE	3.1
28	DF	76	PHE	3.1
6	CG	117	LEU	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
23	DB	2309	A	3.1
45	BY	40	THR	3.1
12	AM	95	PRO	3.1
43	BW	10	ARG	3.1
1	CA	1003	G	3.1
5	CF	46	GLN	3.1
11	AL	111	GLN	3.1
13	CN	77	GLY	3.1
14	AO	34	GLN	3.1
23	BB	978	G	3.1
27	DE	94	GLN	3.1
2	AC	175	HIS	3.1
27	BE	140	ASP	3.1
47	B0	40	HIS	3.1
9	CJ	11	LYS	3.1
27	BE	169	VAL	3.1
27	BE	185	LYS	3.1
52	BI	3	LYS	3.1
35	BN	15	SER	3.1
38	BQ	75	TYR	3.1
47	B0	33	SER	3.1
3	CD	171	GLU	3.1
39	DR	3	ALA	3.1
39	DR	77	PHE	3.1
42	BU	86	PHE	3.1
27	BE	112	LEU	3.1
38	DQ	17	LEU	3.1
42	BU	40	LEU	3.1
27	DE	175	ILE	3.1
33	BL	111	ILE	3.1
34	BM	73	ILE	3.1
27	BE	117	ARG	3.1
27	BE	43	THR	3.1
49	B2	43	THR	3.1
23	DB	1072	C	3.1
24	DV	27	PRO	3.1
38	BQ	22	GLY	3.1
23	BB	13	A	3.1
35	BN	99	LYS	3.1
42	DU	91	LYS	3.1
50	B3	2	LYS	3.1
50	B3	11	LYS	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
36	BO	47	VAL	3.1
21	AU	18	PHE	3.1
23	BB	2319	G	3.1
23	DB	356	G	3.1
35	BN	25	ALA	3.1
36	BO	48	LEU	3.1
52	BI	114	ALA	3.1
19	CT	3	ILE	3.1
22	BA	87	U	3.1
35	DN	33	ILE	3.1
25	DC	13	ARG	3.1
28	DF	124	ARG	3.1
35	BN	73	ASN	3.1
35	DN	45	ARG	3.1
36	DO	96	GLY	3.1
27	BE	1	MET	3.1
41	DT	88	LYS	3.1
50	D3	2	LYS	3.1
22	BA	12	C	3.1
23	DB	11	C	3.1
41	DT	15	HIS	3.1
3	AD	4	LEU	3.1
23	DB	10	A	3.1
23	DB	1275	A	3.1
28	BF	151	LEU	3.1
41	DT	61	LEU	3.1
2	CC	117	ASP	3.1
25	DC	220	ARG	3.1
33	BL	59	ARG	3.1
50	D3	44	ARG	3.1
3	AD	191	SER	3.1
14	AO	1	SER	3.1
26	BD	199	SER	3.1
27	BE	127	GLU	3.1
29	BG	172	GLU	3.1
41	BT	5	GLU	3.1
45	BY	38	GLU	3.1
26	BD	32	ASN	3.1
36	BO	67	ASN	3.1
7	AH	119	GLY	3.1
16	CQ	73	THR	3.1
18	CS	53	GLY	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
40	BS	100	THR	3.1
14	AO	72	LYS	3.1
25	BC	252	LYS	3.1
41	DT	68	LYS	3.1
45	BY	18	LYS	3.1
13	CN	44	VAL	3.1
31	BJ	105	VAL	3.1
36	BO	78	VAL	3.1
37	DP	72	VAL	3.1
33	DL	6	LEU	3.1
34	DM	31	PHE	3.1
38	DQ	13	HIS	3.1
41	BT	32	LEU	3.1
6	AG	3	ARG	3.1
11	CL	25	ALA	3.1
20	AB	20	ARG	3.1
31	DJ	13	ARG	3.1
35	BN	124	ALA	3.1
41	BT	3	ARG	3.1
42	DU	34	ILE	3.1
23	BB	1102	C	3.1
7	CH	53	ASP	3.0
27	DE	116	ASP	3.0
28	BF	142	TYR	3.1
11	AL	69	GLU	3.0
28	BF	31	GLU	3.0
37	DP	111	GLU	3.0
1	CA	466	A	3.0
23	BB	878	A	3.0
23	BB	1073	A	3.0
23	DB	1098	A	3.0
43	BW	29	SER	3.0
31	DJ	39	LYS	3.0
42	DU	43	LYS	3.0
48	B1	3	GLY	3.0
31	DJ	24	THR	3.0
43	BW	42	THR	3.0
23	DB	2585	U	3.0
20	AB	46	VAL	3.0
20	CB	162	VAL	3.0
30	DH	115	VAL	3.0
24	BV	61	LEU	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
26	BD	15	PHE	3.0
41	DT	8	LEU	3.0
43	BW	44	PHE	3.0
45	BY	10	ARG	3.0
51	B4	19	ARG	3.0
11	AL	95	HIS	3.0
28	BF	69	ALA	3.0
32	DK	95	ILE	3.0
34	DM	94	ALA	3.0
52	DI	103	ALA	3.0
25	BC	61	TYR	3.0
27	BE	191	ASP	3.0
34	DM	92	TRP	3.0
39	BR	62	GLU	3.0
15	AP	80	LYS	3.0
25	BC	260	LYS	3.0
26	DD	8	LYS	3.0
38	BQ	4	LYS	3.0
47	B0	52	LYS	3.0
22	DA	68	C	3.0
23	BB	901	C	3.0
33	BL	16	GLY	3.0
41	DT	27	SER	3.0
44	BX	27	ASN	3.0
52	DI	93	ASN	3.0
1	AA	1493	A	3.0
1	CA	747	A	3.0
22	BA	52	A	3.0
25	BC	249	VAL	3.0
27	DE	193	VAL	3.0
30	BH	110	VAL	3.0
39	BR	38	VAL	3.0
12	CM	112	ARG	3.0
26	BD	59	ARG	3.0
33	BL	104	GLN	3.0
34	BM	130	PHE	3.0
37	BP	87	ARG	3.0
41	BT	8	LEU	3.0
42	BU	85	ARG	3.0
43	BW	40	ARG	3.0
46	BZ	60	PHE	3.0
15	AP	43	ALA	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
15	CP	42	ILE	3.0
30	BH	94	ILE	3.0
18	CS	13	HIS	3.0
26	BD	55	LYS	3.0
29	BG	163	TYR	3.0
6	CG	59	GLU	3.0
29	DG	123	GLU	3.0
37	BP	33	GLU	3.0
1	AA	79	G	3.0
6	CG	13	PRO	3.0
23	DB	1087	G	3.0
23	DB	1546	G	3.0
23	DB	2867	G	3.0
27	BE	7	ASP	3.0
34	DM	85	GLY	3.0
47	B0	14	MET	3.0
12	CM	24	VAL	3.0
27	BE	186	VAL	3.0
33	DL	30	THR	3.0
43	BW	11	ASN	3.0
52	DI	131	THR	3.0
42	BU	5	ARG	3.0
47	B0	39	ARG	3.0
52	DI	30	GLN	3.0
3	AD	1	ALA	3.0
23	BB	1057	A	3.0
23	DB	1808	A	3.0
26	BD	102	ALA	3.0
39	BR	27	ILE	3.0
17	CR	73	HIS	3.0
28	DF	4	HIS	3.0
51	B4	27	CYS	3.0
51	D4	27	CYS	3.0
18	CS	69	LYS	3.0
23	BB	646	U	3.0
23	BB	2213	U	3.0
23	DB	102	U	3.0
23	DB	1174	U	3.0
27	BE	137	LYS	3.0
30	DH	112	LYS	3.0
33	DL	29	LYS	3.0
39	BR	71	LYS	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
41	DT	33	LYS	3.0
27	BE	51	GLU	3.0
35	DN	32	GLU	3.0
37	BP	10	GLU	3.0
39	DR	37	GLU	3.0
2	CC	111	ASP	3.0
25	BC	15	VAL	3.0
25	DC	140	VAL	3.0
27	BE	145	ASP	3.0
35	DN	58	ASP	3.0
35	DN	69	ARG	3.0
36	BO	13	ARG	3.0
37	DP	69	VAL	3.0
39	BR	25	LEU	3.0
51	D4	19	ARG	3.0
46	DZ	45	THR	3.0
1	AA	251	G	3.0
24	BV	89	ILE	3.0
24	DV	87	GLN	3.0
29	BG	25	ILE	3.0
35	DN	125	ALA	3.0
40	BS	55	ILE	3.0
52	BI	54	ILE	3.0
14	CO	37	HIS	3.0
16	CQ	15	LYS	3.0
20	CB	131	LYS	3.0
21	AU	19	LYS	3.0
26	DD	159	LYS	3.0
29	BG	175	LYS	3.0
35	BN	121	LYS	3.0
35	BN	100	CYS	3.0
23	DB	846	U	3.0
34	BM	4	PRO	3.0
36	DO	101	GLY	3.0
48	B1	30	PRO	3.0
48	D1	31	GLU	3.0
10	CK	127	ARG	3.0
25	BC	42	ARG	3.0
15	AP	74	LEU	3.0
27	BE	121	VAL	3.0
40	DS	23	LEU	3.0
41	BT	85	VAL	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
28	DF	112	ASP	3.0
6	AG	76	SER	3.0
18	AS	40	PHE	3.0
35	BN	87	PHE	3.0
40	BS	12	SER	3.0
47	B0	25	THR	3.0
48	D1	38	PHE	3.0
3	CD	36	ALA	3.0
6	CG	11	ILE	3.0
27	DE	163	ASN	3.0
34	BM	126	ILE	3.0
48	B1	53	ILE	3.0
4	AE	81	GLN	2.9
39	BR	10	LYS	2.9
39	BR	91	GLN	2.9
41	BT	68	LYS	2.9
1	AA	724	G	2.9
23	BB	2318	G	2.9
23	BB	2458	G	2.9
9	CJ	7	ARG	2.9
18	CS	7	GLY	2.9
35	DN	64	ARG	2.9
47	B0	16	ARG	2.9
23	BB	2103	C	2.9
28	BF	30	VAL	2.9
30	DH	19	VAL	2.9
34	BM	75	GLU	2.9
40	BS	78	GLU	2.9
48	B1	50	GLU	2.9
1	AA	466	A	2.9
23	DB	1420	A	2.9
8	AI	126	PHE	2.9
23	DB	2213	U	2.9
24	BV	91	PHE	2.9
43	DW	59	PHE	2.9
13	AN	30	ILE	2.9
25	BC	245	THR	2.9
25	DC	222	THR	2.9
39	DR	55	ASP	2.9
27	DE	135	ALA	2.9
30	BH	67	ALA	2.9
37	BP	28	LYS	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
37	DP	82	SER	2.9
40	DS	27	LYS	2.9
33	DL	104	GLN	2.9
5	CF	91	ARG	2.9
10	AK	91	GLY	2.9
27	DE	188	MET	2.9
49	D2	12	ARG	2.9
31	BJ	83	GLY	2.9
33	DL	26	GLY	2.9
9	AJ	74	VAL	2.9
25	BC	215	VAL	2.9
28	BF	56	LEU	2.9
28	DF	175	PRO	2.9
30	BH	130	VAL	2.9
38	DQ	94	LEU	2.9
40	DS	45	VAL	2.9
42	DU	33	VAL	2.9
15	CP	77	GLU	2.9
12	CM	21	ILE	2.9
17	AR	38	ILE	2.9
25	DC	58	LYS	2.9
27	BE	6	LYS	2.9
32	BK	77	ILE	2.9
34	DM	96	ILE	2.9
40	DS	66	ILE	2.9
42	DU	71	ILE	2.9
1	CA	447	G	2.9
9	CJ	93	ALA	2.9
19	AT	40	ALA	2.9
23	BB	1072	C	2.9
23	BB	1510	G	2.9
26	BD	47	ALA	2.9
36	DO	37	ALA	2.9
52	BI	113	ALA	2.9
1	AA	88	U	2.9
1	AA	461	A	2.9
1	CA	85	U	2.9
2	CC	182	ASP	2.9
3	CD	28	ASP	2.9
5	AF	41	ASP	2.9
28	BF	5	ASP	2.9
41	BT	21	SER	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
13	CN	42	ASN	2.9
14	CO	61	GLN	2.9
34	BM	88	ASN	2.9
52	BI	30	GLN	2.9
21	CU	32	ARG	2.9
21	CU	44	ARG	2.9
35	BN	8	ARG	2.9
37	BP	76	HIS	2.9
24	BV	1	MET	2.9
26	BD	53	GLY	2.9
37	BP	113	LEU	2.9
37	DP	46	VAL	2.9
52	DI	118	GLY	2.9
27	DE	18	THR	2.9
6	AG	36	SER	2.9
11	AL	46	SER	2.9
19	AT	13	SER	2.9
37	DP	14	GLN	2.9
1	CA	463	U	2.9
23	BB	140	C	2.9
23	BB	546	U	2.9
23	BB	2267	A	2.9
23	DB	143	C	2.9
23	DB	456	C	2.9
23	BB	2286	G	2.9
23	BB	2311	A	2.9
23	DB	1552	A	2.9
23	DB	2310	C	2.9
23	DB	2336	A	2.9
31	DJ	131	ASN	2.9
25	DC	131	MET	2.9
27	DE	134	LEU	2.9
52	DI	10	LEU	2.9
4	AE	113	VAL	2.9
31	DJ	64	VAL	2.9
40	BS	80	PRO	2.9
13	AN	46	LYS	2.9
26	BD	159	LYS	2.9
41	BT	64	LYS	2.9
16	CQ	25	GLU	2.9
18	CS	10	ILE	2.9
27	BE	111	GLU	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	DM	130	PHE	2.9
52	BI	66	PHE	2.9
52	DI	129	GLU	2.9
31	DJ	117	ALA	2.9
21	AU	41	THR	2.9
25	DC	166	ARG	2.9
34	DM	66	ARG	2.9
26	DD	95	SER	2.9
31	BJ	25	LEU	2.9
39	DR	22	LEU	2.9
47	B0	26	SER	2.9
42	BU	44	HIS	2.9
25	BC	46	GLY	2.9
26	DD	76	GLY	2.9
30	BH	9	VAL	2.9
42	DU	73	ASN	2.9
42	BU	54	PRO	2.9
23	BB	1348	C	2.9
47	B0	47	TYR	2.9
28	BF	137	PHE	2.9
1	AA	1002	G	2.8
23	DB	1051	G	2.8
26	DD	99	GLU	2.8
30	DH	76	GLU	2.8
50	D3	64	ALA	2.8
52	BI	17	ALA	2.8
3	AD	62	ARG	2.8
18	CS	77	ARG	2.8
43	DW	38	ARG	2.8
28	DF	34	THR	2.8
31	BJ	70	THR	2.8
33	BL	74	THR	2.8
35	DN	57	THR	2.8
27	DE	12	LEU	2.8
8	CI	103	VAL	2.8
11	CL	88	ASP	2.8
36	DO	19	GLN	2.8
52	DI	11	GLN	2.8
25	DC	4	LYS	2.8
25	DC	138	SER	2.8
33	BL	129	LYS	2.8
37	BP	55	HIS	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
37	BP	105	LYS	2.8
43	DW	22	VAL	2.8
3	AD	6	PRO	2.8
9	AJ	41	PRO	2.8
13	AN	20	PHE	2.8
20	AB	68	PHE	2.8
36	BO	87	ILE	2.8
42	DU	57	ILE	2.8
2	CC	70	ALA	2.8
3	AD	34	GLU	2.8
23	BB	846	U	2.8
34	BM	116	ALA	2.8
38	BQ	95	ALA	2.8
43	BW	83	ALA	2.8
1	CA	1226	C	2.8
23	BB	877	A	2.8
36	BO	30	ARG	2.8
23	BB	1092	C	2.8
23	DB	1178	C	2.8
13	CN	50	LEU	2.8
15	CP	52	LEU	2.8
28	DF	67	THR	2.8
47	B0	32	THR	2.8
32	BK	20	MET	2.8
1	CA	993	G	2.8
15	CP	13	LYS	2.8
25	BC	255	LYS	2.8
31	BJ	39	LYS	2.8
7	AH	17	GLN	2.8
7	AH	121	GLY	2.8
8	AI	101	GLY	2.8
43	DW	14	ASP	2.8
25	DC	28	PRO	2.8
36	DO	8	ILE	2.8
41	BT	30	ILE	2.8
42	BU	64	ILE	2.8
28	BF	6	TYR	2.8
31	BJ	15	TRP	2.8
37	BP	30	TRP	2.8
5	AF	99	ALA	2.8
20	CB	34	ARG	2.8
26	BD	69	ALA	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
31	BJ	94	ALA	2.8
33	BL	21	ARG	2.8
50	B3	59	ALA	2.8
51	B4	24	ARG	2.8
4	CE	115	GLU	2.8
23	BB	4	U	2.8
23	BB	1082	U	2.8
23	DB	1101	U	2.8
18	CS	4	LEU	2.8
27	BE	134	LEU	2.8
30	DH	30	LEU	2.8
12	CM	26	LYS	2.8
25	DC	6	LYS	2.8
29	BG	159	LYS	2.8
34	BM	133	LYS	2.8
38	DQ	18	LYS	2.8
1	CA	1285	A	2.8
2	CC	105	VAL	2.8
23	BB	1525	A	2.8
24	BV	72	VAL	2.8
27	BE	113	VAL	2.8
27	BE	187	VAL	2.8
29	DG	16	VAL	2.8
48	D1	17	GLY	2.8
25	DC	7	PRO	2.8
34	DM	117	PHE	2.8
44	BX	26	PHE	2.8
46	DZ	42	PRO	2.8
9	AJ	91	ASP	2.8
29	DG	165	ASP	2.8
39	BR	7	SER	2.8
42	DU	29	SER	2.8
1	AA	1432	G	2.8
20	AB	82	ALA	2.8
23	BB	1699	G	2.8
25	BC	20	ASN	2.8
35	DN	96	ARG	2.8
30	BH	84	ALA	2.8
27	DE	51	GLU	2.8
31	BJ	98	GLU	2.8
15	AP	6	LEU	2.8
27	DE	98	LYS	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
27	DE	112	LEU	2.8
27	DE	143	LEU	2.8
34	DM	102	LEU	2.8
36	BO	106	LEU	2.8
47	B0	56	LYS	2.8
28	DF	37	MET	2.8
33	BL	1	MET	2.8
25	BC	194	VAL	2.8
25	DC	267	VAL	2.8
33	BL	118	THR	2.8
34	DM	128	THR	2.8
10	CK	119	GLY	2.8
25	BC	148	GLY	2.8
28	DF	38	GLY	2.8
39	DR	56	GLY	2.8
43	DW	64	GLY	2.8
5	CF	51	ILE	2.8
12	AM	11	HIS	2.8
15	AP	39	PHE	2.8
18	AS	51	HIS	2.8
20	CB	169	HIS	2.8
25	DC	52	HIS	2.8
39	DR	89	HIS	2.8
18	AS	8	PRO	2.8
1	AA	199	A	2.8
23	BB	1552	A	2.8
9	CJ	97	ASP	2.8
18	CS	74	ALA	2.8
20	CB	52	ALA	2.8
25	BC	165	ALA	2.8
26	BD	196	ALA	2.8
27	BE	39	ALA	2.8
41	DT	13	ALA	2.8
43	BW	5	ALA	2.8
46	DZ	38	SER	2.8
47	D0	26	SER	2.8
52	BI	76	ALA	2.8
3	AD	87	GLU	2.8
5	AF	98	GLU	2.8
25	BC	206	LYS	2.8
33	BL	106	GLU	2.8
13	CN	5	MET	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
26	BD	172	VAL	2.8
27	DE	113	VAL	2.8
38	DQ	99	VAL	2.8
39	DR	72	VAL	2.8
41	BT	10	VAL	2.8
1	CA	812	G	2.8
23	BB	974	G	2.8
9	CJ	44	THR	2.8
12	CM	107	THR	2.8
33	BL	30	THR	2.8
52	BI	111	THR	2.8
39	DR	9	GLY	2.8
12	CM	6	ILE	2.8
26	BD	173	GLN	2.7
28	BF	76	PHE	2.8
29	DG	169	ARG	2.7
31	DJ	93	ILE	2.8
9	CJ	61	ALA	2.7
33	DL	98	ALA	2.7
36	BO	11	ALA	2.7
9	AJ	19	ASP	2.7
15	AP	69	ASP	2.7
35	DN	89	SER	2.7
36	BO	4	LYS	2.7
42	BU	80	ASP	2.7
43	BW	55	ASP	2.7
43	DW	23	LYS	2.7
49	D2	8	SER	2.7
23	BB	101	A	2.7
23	DB	1089	A	2.7
43	BW	49	ASN	2.7
26	BD	178	VAL	2.7
31	BJ	62	VAL	2.7
37	DP	91	VAL	2.7
9	CJ	95	GLY	2.7
14	AO	63	ARG	2.7
26	DD	12	THR	2.7
16	CQ	27	PHE	2.7
20	AB	49	PHE	2.7
28	BF	136	ILE	2.7
31	DJ	3	THR	2.7
34	BM	10	ARG	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
52	BI	133	ARG	2.7
9	AJ	56	HIS	2.7
14	CO	45	HIS	2.7
29	BG	153	PRO	2.7
52	DI	22	PRO	2.7
1	AA	377	G	2.7
1	AA	450	G	2.7
9	AJ	82	LYS	2.7
23	DB	2780	G	2.7
40	DS	98	LYS	2.7
45	BY	2	LYS	2.7
20	CB	100	LEU	2.7
23	DB	1458	U	2.7
26	BD	80	TRP	2.7
34	BM	95	LEU	2.7
38	DQ	44	TYR	2.7
43	BW	20	LEU	2.7
44	BX	19	LEU	2.7
52	BI	65	SER	2.7
8	CI	18	VAL	2.7
13	CN	33	VAL	2.7
20	AB	117	GLU	2.7
26	DD	170	VAL	2.7
41	DT	89	GLU	2.7
23	BB	1086	A	2.7
33	DL	41	ARG	2.7
4	AE	128	GLY	2.7
29	BG	140	ILE	2.7
30	BH	72	ILE	2.7
32	BK	39	ILE	2.7
52	DI	58	ILE	2.7
11	AL	119	LYS	2.7
15	AP	9	HIS	2.7
31	DJ	137	PRO	2.7
3	AD	148	ALA	2.7
12	CM	34	ALA	2.7
19	AT	70	LYS	2.7
34	DM	8	LYS	2.7
39	BR	81	LYS	2.7
43	BW	32	ALA	2.7
50	D3	26	ALA	2.7
52	DI	13	ALA	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
26	BD	186	LEU	2.7
28	DF	90	LEU	2.7
40	BS	69	LEU	2.7
36	BO	99	TYR	2.7
52	BI	7	TYR	2.7
26	DD	1	MET	2.7
52	BI	16	MET	2.7
26	DD	172	VAL	2.7
23	BB	2180	U	2.7
34	DM	70	ASP	2.7
38	BQ	86	SER	2.7
1	AA	220	G	2.7
1	CA	1032	G	2.7
23	BB	2136	G	2.7
23	BB	2801	G	2.7
23	BB	2808	G	2.7
36	BO	80	GLU	2.7
27	DE	88	ARG	2.7
31	DJ	34	ARG	2.7
13	AN	94	GLY	2.7
25	BC	137	GLY	2.7
26	BD	2	ILE	2.7
31	DJ	26	GLY	2.7
33	BL	142	ILE	2.7
38	BQ	79	ILE	2.7
43	BW	25	PHE	2.7
46	DZ	64	PHE	2.7
13	AN	11	LYS	2.7
23	BB	1088	A	2.7
23	DB	1073	A	2.7
34	BM	14	LYS	2.7
36	BO	63	LYS	2.7
50	B3	38	LYS	2.7
6	AG	21	LEU	2.7
11	AL	23	LEU	2.7
23	BB	2023	C	2.7
23	DB	1075	C	2.7
26	DD	138	LEU	2.7
39	DR	25	LEU	2.7
51	B4	37	GLN	2.7
8	CI	63	TYR	2.7
11	CL	37	TYR	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
28	BF	24	VAL	2.7
3	CD	2	ARG	2.7
16	CQ	26	ARG	2.7
38	DQ	10	ARG	2.7
44	BX	47	ARG	2.7
25	BC	138	SER	2.7
27	BE	171	ASP	2.7
37	BP	35	SER	2.7
52	BI	129	GLU	2.7
2	CC	74	ILE	2.7
3	AD	194	ILE	2.7
25	DC	225	ASN	2.7
27	DE	73	ILE	2.7
41	DT	30	ILE	2.7
23	DB	1340	U	2.7
25	DC	40	GLY	2.7
26	BD	93	GLY	2.7
35	BN	102	PHE	2.7
36	BO	44	GLY	2.7
37	DP	58	PHE	2.7
11	CL	87	LYS	2.7
35	BN	5	LYS	2.7
41	DT	64	LYS	2.7
3	AD	45	PRO	2.7
6	AG	15	PRO	2.7
26	DD	35	THR	2.7
31	DJ	65	THR	2.7
45	BY	9	THR	2.7
10	AK	41	LEU	2.7
11	AL	25	ALA	2.7
27	DE	133	LEU	2.7
28	BF	116	LEU	2.7
29	BG	39	ALA	2.7
30	DH	148	ALA	2.7
41	DT	99	ALA	2.7
43	DW	83	ALA	2.7
38	BQ	55	GLN	2.7
44	BX	1	MET	2.7
2	CC	41	TYR	2.7
28	BF	73	VAL	2.7
28	BF	82	TYR	2.7
32	BK	35	VAL	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
47	D0	47	TYR	2.7
23	BB	1076	C	2.7
25	DC	261	ARG	2.7
37	DP	20	ARG	2.7
12	AM	20	SER	2.6
17	AR	19	GLU	2.6
34	BM	115	GLU	2.6
37	DP	63	ILE	2.6
37	DP	67	GLU	2.6
39	DR	34	GLU	2.6
41	BT	74	ILE	2.6
52	BI	34	ILE	2.6
2	AC	154	GLY	2.6
6	AG	7	GLY	2.6
6	AG	150	PHE	2.6
9	AJ	75	ASP	2.6
12	AM	43	LYS	2.6
13	AN	72	PHE	2.6
13	CN	46	LYS	2.6
25	BC	56	GLY	2.6
27	DE	58	LYS	2.6
28	DF	115	GLY	2.6
29	DG	160	GLY	2.6
31	BJ	82	GLY	2.6
32	BK	53	LYS	2.6
33	DL	65	GLY	2.6
37	BP	22	GLY	2.6
39	BR	26	ASP	2.6
43	BW	78	PHE	2.6
45	DY	32	GLY	2.6
51	B4	15	LYS	2.6
52	BI	37	PHE	2.6
35	DN	11	ASN	2.6
12	AM	9	PRO	2.6
12	AM	55	LEU	2.6
18	CS	32	THR	2.6
23	BB	138	U	2.6
27	DE	46	GLN	2.6
41	DT	72	GLN	2.6
13	AN	40	ARG	2.6
38	BQ	29	ARG	2.6
40	DS	84	ARG	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
48	B1	46	VAL	2.6
47	B0	48	TYR	2.6
1	AA	1491	G	2.6
23	BB	1093	G	2.6
23	DB	1056	G	2.6
23	DB	2107	G	2.6
19	AT	66	ILE	2.6
36	BO	40	ILE	2.6
2	AC	158	GLY	2.6
11	AL	83	GLY	2.6
16	AQ	27	PHE	2.6
30	DH	60	GLU	2.6
35	DN	100	CYS	2.6
39	DR	88	GLY	2.6
46	DZ	44	PHE	2.6
49	D2	38	GLY	2.6
52	BI	49	GLU	2.6
16	AQ	14	ASP	2.6
20	AB	126	ASP	2.6
30	DH	86	ASP	2.6
37	BP	23	ASP	2.6
45	BY	51	SER	2.6
31	DJ	8	PRO	2.6
34	BM	113	ALA	2.6
38	BQ	71	ASN	2.6
38	DQ	108	LEU	2.6
44	BX	6	LEU	2.6
25	BC	31	PRO	2.6
25	DC	121	ALA	2.6
36	BO	32	PRO	2.6
47	B0	5	ASN	2.6
48	B1	51	ALA	2.6
26	BD	25	THR	2.6
46	BZ	41	HIS	2.6
52	DI	16	MET	2.6
25	DC	202	ARG	2.6
26	BD	77	ARG	2.6
28	BF	70	ARG	2.6
30	BH	68	ARG	2.6
34	DM	6	ARG	2.6
43	DW	13	ARG	2.6
33	BL	85	VAL	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	BL	120	VAL	2.6
4	CE	127	TYR	2.6
29	BG	171	LYS	2.6
34	DM	84	LYS	2.6
43	DW	61	LYS	2.6
48	D1	2	LYS	2.6
52	BI	81	LYS	2.6
25	BC	265	PHE	2.6
43	DW	78	PHE	2.6
6	AG	39	GLU	2.6
11	AL	68	GLY	2.6
19	AT	64	GLY	2.6
25	DC	248	GLY	2.6
26	BD	86	GLU	2.6
27	DE	197	GLU	2.6
33	DL	144	GLU	2.6
9	CJ	73	LEU	2.6
12	AM	79	LEU	2.6
31	DJ	25	LEU	2.6
49	D2	42	LEU	2.6
1	CA	373	A	2.6
13	AN	86	ALA	2.6
19	CT	6	ALA	2.6
23	BB	142	A	2.6
23	DB	1913	A	2.6
1	AA	212	G	2.6
1	CA	413	G	2.6
23	BB	1154	G	2.6
23	BB	2156	G	2.6
29	BG	53	PRO	2.6
52	BI	21	PRO	2.6
26	DD	42	ASN	2.6
44	DX	15	ASN	2.6
52	BI	33	ASN	2.6
6	AG	137	ARG	2.6
11	CL	8	ARG	2.6
27	DE	49	ARG	2.6
31	BJ	3	THR	2.6
46	DZ	25	ARG	2.6
39	BR	20	VAL	2.6
2	CC	2	GLN	2.6
2	CC	21	TRP	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	DK	67	LYS	2.6
38	BQ	60	TRP	2.6
42	BU	43	LYS	2.6
1	AA	534	U	2.6
1	AA	1240	U	2.6
23	BB	1058	U	2.6
23	BB	1584	U	2.6
39	DR	8	GLY	2.6
33	BL	10	GLU	2.6
37	BP	101	GLU	2.6
4	AE	124	ALA	2.6
20	CB	159	ALA	2.6
24	BV	37	PRO	2.6
34	DM	98	PRO	2.6
35	DN	122	ALA	2.6
3	CD	72	ARG	2.6
9	CJ	68	ARG	2.6
26	BD	108	ASP	2.6
27	BE	116	ASP	2.6
45	BY	53	MET	2.6
46	BZ	58	ASP	2.6
48	D1	5	ARG	2.6
19	CT	57	VAL	2.6
32	DK	122	VAL	2.6
36	DO	54	VAL	2.6
44	DX	41	HIS	2.6
1	AA	80	A	2.6
23	BB	508	A	2.6
23	DB	1395	A	2.6
26	BD	204	LYS	2.6
49	B2	11	LYS	2.6
25	BC	59	GLN	2.6
27	DE	195	GLN	2.6
38	BQ	19	GLN	2.6
38	DQ	55	GLN	2.6
44	DX	38	GLN	2.6
22	DA	69	G	2.6
23	BB	331	C	2.6
23	BB	2150	C	2.6
23	DB	1093	G	2.6
37	BP	47	ILE	2.6
37	DP	83	ILE	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
46	DZ	5	ILE	2.6
7	AH	64	TYR	2.6
37	BP	19	PHE	2.6
39	BR	53	PHE	2.6
4	CE	90	GLY	2.6
15	CP	30	GLY	2.6
26	DD	153	GLY	2.6
30	DH	75	LEU	2.6
36	BO	66	GLY	2.6
43	BW	31	LEU	2.6
52	BI	84	GLY	2.6
26	BD	74	GLU	2.6
11	AL	27	PRO	2.6
11	CL	121	PRO	2.6
18	CS	80	ARG	2.6
27	DE	45	ALA	2.6
29	DG	173	ALA	2.6
30	BH	50	ARG	2.6
33	DL	2	ARG	2.6
33	DL	137	ALA	2.6
49	B2	35	ARG	2.6
21	AU	24	LYS	2.6
25	BC	171	VAL	2.6
25	DC	15	VAL	2.6
25	DC	249	VAL	2.6
30	BH	103	VAL	2.6
33	DL	36	LYS	2.6
37	BP	85	VAL	2.6
41	DT	34	VAL	2.6
12	CM	104	ASN	2.6
18	AS	38	THR	2.6
37	DP	23	ASP	2.6
36	DO	67	ASN	2.6
40	BS	3	THR	2.6
42	DU	52	ASN	2.6
5	AF	6	ILE	2.5
37	BP	83	ILE	2.5
39	DR	27	ILE	2.5
47	B0	54	ILE	2.5
1	AA	81	A	2.5
1	AA	814	A	2.5
1	CA	412	A	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
21	AU	28	LEU	2.5
23	BB	2406	A	2.5
23	DB	1080	A	2.5
23	DB	1086	A	2.5
24	DV	38	LEU	2.5
26	DD	100	LEU	2.5
28	DF	82	TYR	2.5
33	BL	11	GLY	2.5
33	BL	124	GLY	2.5
42	DU	31	GLY	2.5
20	AB	208	ALA	2.5
30	DH	23	ALA	2.5
33	DL	132	ARG	2.5
34	DM	21	ALA	2.5
48	D1	27	ARG	2.5
1	AA	94	G	2.5
21	AU	10	PRO	2.5
23	BB	45	G	2.5
23	BB	726	G	2.5
46	BZ	42	PRO	2.5
1	AA	1364	U	2.5
16	CQ	82	VAL	2.5
23	BB	1458	U	2.5
25	DC	17	LYS	2.5
27	DE	83	VAL	2.5
29	BG	174	LYS	2.5
21	CU	42	THR	2.5
25	BC	141	HIS	2.5
29	BG	55	ASP	2.5
33	BL	5	THR	2.5
47	D0	19	ASP	2.5
2	CC	161	ILE	2.5
13	CN	30	ILE	2.5
28	BF	22	ASN	2.5
31	BJ	103	ILE	2.5
3	AD	70	GLN	2.5
3	AD	151	GLN	2.5
27	BE	41	GLN	2.5
27	DE	41	GLN	2.5
13	AN	15	LEU	2.5
26	BD	4	LEU	2.5
42	DU	86	PHE	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	AD	75	TYR	2.5
25	DC	170	TYR	2.5
44	DX	62	GLY	2.5
46	BZ	29	GLY	2.5
6	CG	108	ARG	2.5
27	BE	61	ARG	2.5
27	DE	67	ARG	2.5
28	DF	79	ARG	2.5
38	DQ	2	ARG	2.5
45	BY	29	ARG	2.5
31	DJ	63	ALA	2.5
34	DM	122	ALA	2.5
42	BU	74	ALA	2.5
50	B3	47	ALA	2.5
1	AA	1333	A	2.5
3	AD	162	GLU	2.5
4	AE	115	GLU	2.5
13	CN	22	LYS	2.5
26	BD	7	LYS	2.5
31	BJ	31	GLU	2.5
34	BM	123	LYS	2.5
34	DM	72	PRO	2.5
37	DP	93	LYS	2.5
39	DR	60	LYS	2.5
42	BU	42	LYS	2.5
41	BT	16	VAL	2.5
1	AA	578	C	2.5
23	BB	2109	U	2.5
23	BB	2155	U	2.5
23	DB	276	U	2.5
23	DB	2109	U	2.5
29	BG	170	THR	2.5
33	BL	94	THR	2.5
35	BN	75	ILE	2.5
37	DP	84	SER	2.5
45	DY	4	ILE	2.5
52	BI	108	ILE	2.5
23	DB	1910	G	2.5
52	BI	38	CYS	2.5
52	BI	47	SER	2.5
29	DG	136	ASP	2.5
8	CI	109	GLN	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
31	DJ	122	LEU	2.5
32	BK	25	LEU	2.5
48	B1	44	GLN	2.5
15	CP	10	GLY	2.5
31	BJ	53	TYR	2.5
31	DJ	74	TYR	2.5
34	DM	44	ARG	2.5
43	BW	51	GLY	2.5
4	AE	138	ALA	2.5
14	AO	47	LYS	2.5
21	CU	24	LYS	2.5
25	BC	111	ALA	2.5
26	DD	55	LYS	2.5
35	BN	61	ALA	2.5
36	BO	68	LYS	2.5
9	CJ	57	VAL	2.5
16	AQ	62	GLU	2.5
25	DC	143	VAL	2.5
26	BD	73	VAL	2.5
33	DL	8	PRO	2.5
30	BH	149	GLU	2.5
39	BR	47	VAL	2.5
42	BU	27	VAL	2.5
1	AA	1014	A	2.5
23	BB	1095	A	2.5
23	BB	1098	A	2.5
23	DB	899	A	2.5
12	AM	52	ILE	2.5
40	BS	7	HIS	2.5
42	BU	102	ILE	2.5
52	BI	48	ILE	2.5
13	CN	20	PHE	2.5
20	CB	178	LEU	2.5
24	BV	3	THR	2.5
25	BC	262	THR	2.5
34	BM	129	THR	2.5
36	BO	115	LEU	2.5
14	CO	57	ARG	2.5
22	BA	118	C	2.5
26	BD	97	SER	2.5
39	BR	35	PHE	2.5
32	BK	21	CYS	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	DK	73	ASP	2.5
33	BL	41	ARG	2.5
1	AA	1183	U	2.5
11	AL	4	ASN	2.5
23	BB	1340	U	2.5
23	BB	2797	U	2.5
23	DB	1081	U	2.5
23	DB	2372	U	2.5
26	DD	32	ASN	2.5
35	BN	13	ASN	2.5
42	DU	26	ASN	2.5
3	AD	121	ALA	2.5
5	CF	53	LYS	2.5
8	CI	5	TYR	2.5
33	DL	16	GLY	2.5
34	BM	23	GLY	2.5
12	AM	102	LYS	2.5
16	CQ	38	LYS	2.5
33	BL	63	LYS	2.5
38	BQ	9	ALA	2.5
38	DQ	112	ALA	2.5
42	DU	16	LYS	2.5
43	DW	77	LYS	2.5
45	BY	12	ALA	2.5
46	BZ	3	LYS	2.5
1	CA	1006	G	2.5
23	DB	1179	G	2.5
23	DB	2458	G	2.5
50	D3	48	MET	2.5
12	AM	96	VAL	2.5
12	AM	111	PRO	2.5
25	DC	243	PRO	2.5
46	DZ	7	PRO	2.5
51	B4	22	VAL	2.5
52	BI	55	PRO	2.5
6	CG	39	GLU	2.5
26	DD	28	GLU	2.5
35	DN	113	ILE	2.5
3	AD	81	LEU	2.5
12	CM	92	ARG	2.5
28	DF	174	PHE	2.5
20	CB	129	THR	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
26	BD	52	THR	2.5
26	DD	16	THR	2.5
31	BJ	96	ARG	2.5
42	DU	93	ARG	2.5
45	DY	30	ARG	2.5
52	BI	117	THR	2.5
1	AA	60	A	2.5
23	BB	2062	A	2.5
2	CC	153	SER	2.5
10	AK	50	GLY	2.5
10	AK	87	GLY	2.5
25	DC	87	SER	2.5
20	AB	122	ASP	2.5
25	DC	124	LYS	2.5
26	DD	93	GLY	2.5
32	DK	5	GLN	2.5
38	DQ	15	LYS	2.5
41	BT	72	GLN	2.5
40	DS	109	ASP	2.5
43	BW	6	GLY	2.5
50	D3	51	LYS	2.5
52	BI	104	GLN	2.5
52	DI	134	SER	2.5
25	BC	259	ASN	2.5
28	DF	36	ASN	2.5
30	BH	20	ASN	2.5
34	DM	88	ASN	2.5
8	AI	15	ALA	2.5
30	BH	148	ALA	2.5
33	BL	137	ALA	2.5
33	DL	15	ALA	2.5
50	B3	36	ALA	2.5
52	BI	43	ALA	2.5
1	AA	106	C	2.5
23	BB	2185	U	2.5
23	DB	137	U	2.5
28	BF	129	MET	2.5
52	DI	116	MET	2.5
6	AG	79	VAL	2.5
11	CL	15	VAL	2.5
26	DD	92	VAL	2.5
29	DG	14	VAL	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	DM	89	VAL	2.5
39	DR	4	VAL	2.5
39	DR	20	VAL	2.5
9	CJ	39	PRO	2.5
52	DI	25	PRO	2.5
20	AB	128	LEU	2.4
23	BB	2144	G	2.4
23	BB	2885	G	2.4
23	DB	2308	G	2.4
28	DF	109	ARG	2.4
33	DL	126	ARG	2.4
38	BQ	13	HIS	2.4
3	AD	7	LYS	2.4
3	AD	147	LYS	2.4
6	CG	24	LYS	2.4
29	BG	50	THR	2.4
29	DG	170	THR	2.4
48	B1	23	THR	2.4
51	D4	2	LYS	2.4
7	AH	122	GLY	2.4
8	AI	125	GLN	2.4
24	DV	32	GLY	2.4
36	BO	96	GLY	2.4
37	BP	104	GLY	2.4
42	DU	15	GLY	2.4
7	AH	115	ALA	2.4
25	DC	207	ALA	2.4
29	DG	58	ALA	2.4
34	BM	82	MET	2.4
49	D2	36	ALA	2.4
52	BI	35	MET	2.4
52	DI	62	ALA	2.4
1	CA	460	A	2.4
10	CK	19	VAL	2.4
25	DC	44	ASN	2.4
22	BA	66	A	2.4
23	DB	2297	A	2.4
27	BE	14	VAL	2.4
32	BK	84	CYS	2.4
37	BP	51	ASN	2.4
47	B0	29	VAL	2.4
50	B3	27	ASN	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
52	BI	97	VAL	2.4
13	AN	69	PRO	2.4
30	DH	38	PRO	2.4
36	DO	42	PRO	2.4
1	AA	87	C	2.4
4	CE	28	ARG	2.4
9	CJ	45	ARG	2.4
20	CB	213	LEU	2.4
23	BB	527	C	2.4
23	BB	1536	C	2.4
28	DF	33	ILE	2.4
32	BK	2	ILE	2.4
34	DM	126	ILE	2.4
37	DP	109	ILE	2.4
41	BT	69	ARG	2.4
41	DT	4	GLU	2.4
47	D0	54	ILE	2.4
24	BV	38	LEU	2.4
25	BC	86	ARG	2.4
27	BE	44	ARG	2.4
29	BG	34	ARG	2.4
35	DN	90	ARG	2.4
46	BZ	25	ARG	2.4
47	D0	39	ARG	2.4
38	BQ	100	PHE	2.4
9	CJ	70	HIS	2.4
20	CB	104	LYS	2.4
46	BZ	30	HIS	2.4
36	DO	31	THR	2.4
40	DS	100	THR	2.4
19	CT	62	ALA	2.4
25	DC	91	ALA	2.4
25	DC	116	GLN	2.4
35	BN	122	ALA	2.4
43	BW	39	GLN	2.4
46	DZ	52	ALA	2.4
50	D3	47	ALA	2.4
1	AA	1020	G	2.4
3	AD	52	VAL	2.4
4	AE	99	SER	2.4
6	AG	53	SER	2.4
20	AB	13	VAL	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
20	AB	91	VAL	2.4
23	DB	1699	G	2.4
28	BF	39	VAL	2.4
29	DG	112	VAL	2.4
34	DM	27	SER	2.4
39	DR	75	VAL	2.4
43	BW	34	SER	2.4
52	DI	127	SER	2.4
7	CH	5	PRO	2.4
11	CL	90	PRO	2.4
25	BC	10	PRO	2.4
29	DG	11	PRO	2.4
41	DT	92	ASN	2.4
13	CN	73	LEU	2.4
20	AB	9	LEU	2.4
30	DH	94	ILE	2.4
38	BQ	10	ARG	2.4
39	DR	79	ARG	2.4
42	BU	4	ILE	2.4
47	B0	15	ARG	2.4
1	AA	353	A	2.4
1	AA	729	A	2.4
1	AA	1239	A	2.4
23	DB	1048	A	2.4
23	DB	1525	A	2.4
23	DB	2602	A	2.4
34	BM	104	GLU	2.4
1	CA	1301	U	2.4
11	AL	42	LYS	2.4
13	AN	27	LYS	2.4
28	DF	8	LYS	2.4
35	DN	87	PHE	2.4
40	BS	6	LYS	2.4
23	BB	145	C	2.4
23	DB	1100	C	2.4
2	AC	166	TRP	2.4
3	AD	29	THR	2.4
26	DD	87	GLY	2.4
35	BN	53	THR	2.4
41	BT	65	GLY	2.4
27	DE	141	MET	2.4
28	BF	1	ALA	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
29	DG	95	ALA	2.4
32	DK	16	ALA	2.4
34	DM	136	MET	2.4
49	B2	20	ALA	2.4
25	BC	16	VAL	2.4
25	DC	162	GLN	2.4
37	BP	72	VAL	2.4
28	BF	7	TYR	2.4
36	DO	64	TYR	2.4
3	AD	143	SER	2.4
7	CH	1	SER	2.4
10	AK	25	SER	2.4
46	BZ	15	SER	2.4
52	BI	73	PRO	2.4
52	DI	101	SER	2.4
16	AQ	66	LEU	2.4
25	BC	120	ASP	2.4
25	DC	259	ASN	2.4
30	DH	98	ASP	2.4
35	DN	10	LEU	2.4
35	DN	46	ARG	2.4
38	BQ	73	ILE	2.4
25	BC	5	CYS	2.4
3	CD	30	LYS	2.4
16	AQ	3	LYS	2.4
17	CR	23	LYS	2.4
20	AB	10	LYS	2.4
44	BX	2	LYS	2.4
1	AA	111	G	2.4
1	AA	1529	G	2.4
1	CA	203	G	2.4
9	AJ	49	PHE	2.4
23	BB	1055	G	2.4
23	BB	1546	G	2.4
23	BB	1734	G	2.4
24	BV	41	GLU	2.4
28	DF	10	GLU	2.4
1	AA	728	A	2.4
1	AA	1213	A	2.4
1	CA	250	A	2.4
25	BC	14	HIS	2.4
27	DE	29	HIS	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
20	AB	12	GLY	2.4
23	BB	1917	U	2.4
23	DB	12	U	2.4
26	BD	158	GLY	2.4
36	DO	44	GLY	2.4
25	DC	128	THR	2.4
26	DD	54	ALA	2.4
27	BE	161	ALA	2.4
27	BE	192	ALA	2.4
39	DR	29	THR	2.4
52	BI	67	THR	2.4
25	BC	164	VAL	2.4
26	DD	5	VAL	2.4
30	DH	110	VAL	2.4
36	DO	103	VAL	2.4
51	B4	17	VAL	2.4
1	AA	217	C	2.4
1	CA	381	C	2.4
3	AD	80	ARG	2.4
27	BE	67	ARG	2.4
33	DL	78	ARG	2.4
37	DP	78	PRO	2.4
46	BZ	49	ARG	2.4
6	CG	46	LEU	2.4
7	AH	125	ILE	2.4
9	AJ	92	LEU	2.4
20	AB	100	LEU	2.4
30	DH	131	SER	2.4
34	BM	78	LEU	2.4
40	BS	101	SER	2.4
21	AU	4	LYS	2.4
34	BM	71	LYS	2.4
34	DM	100	LYS	2.4
30	DH	28	ASN	2.4
4	CE	30	PHE	2.4
52	DI	37	PHE	2.4
3	AD	112	GLU	2.4
13	CN	85	GLU	2.4
26	BD	28	GLU	2.4
30	BH	70	GLU	2.4
36	DO	20	GLU	2.4
40	DS	59	GLU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
43	BW	16	GLU	2.4
14	CO	50	HIS	2.4
14	AO	33	ALA	2.4
52	DI	75	ALA	2.4
2	AC	75	VAL	2.4
20	CB	209	VAL	2.4
1	CA	86	G	2.4
1	CA	1300	G	2.4
22	DA	24	G	2.4
23	BB	914	G	2.4
23	BB	1737	G	2.4
23	BB	2848	G	2.4
23	DB	1212	G	2.4
23	DB	1524	G	2.4
27	BE	189	THR	2.4
37	BP	91	VAL	2.4
42	DU	48	VAL	2.4
1	AA	109	A	2.4
1	AA	1017	U	2.4
1	AA	1029	U	2.4
1	AA	1111	A	2.4
1	CA	487	A	2.4
3	CD	164	ARG	2.4
8	CI	40	ARG	2.4
12	AM	89	ARG	2.4
23	BB	654	A	2.4
25	DC	237	ARG	2.4
32	BK	78	ARG	2.4
34	DM	3	GLN	2.4
39	BR	87	GLN	2.4
12	CM	22	TYR	2.3
25	DC	25	LYS	2.3
26	BD	62	LYS	2.3
27	BE	175	ILE	2.3
28	BF	105	ILE	2.3
30	BH	5	LEU	2.3
30	BH	8	LYS	2.3
33	DL	105	ILE	2.3
38	DQ	23	TYR	2.3
48	D1	53	ILE	2.3
49	B2	46	LYS	2.3
6	CG	124	SER	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
26	DD	139	SER	2.3
4	CE	69	ASN	2.3
8	AI	61	ASP	2.3
16	CQ	14	ASP	2.3
23	BB	1075	C	2.3
23	DB	1211	C	2.3
30	BH	11	ASN	2.3
34	BM	106	ASP	2.3
42	BU	17	ASP	2.3
42	BU	39	ASN	2.3
52	BI	115	ASP	2.3
21	CU	38	GLU	2.3
34	DM	75	GLU	2.3
43	DW	82	GLU	2.3
10	AK	44	ALA	2.3
19	CT	71	ALA	2.3
30	BH	147	VAL	2.3
30	DH	61	VAL	2.3
32	DK	119	ALA	2.3
46	BZ	36	VAL	2.3
8	CI	83	THR	2.3
38	DQ	54	ARG	2.3
19	AT	4	LYS	2.3
26	BD	40	LEU	2.3
30	BH	15	LEU	2.3
34	BM	100	LYS	2.3
38	BQ	14	LYS	2.3
45	BY	16	LEU	2.3
40	DS	4	ILE	2.3
49	B2	37	LYS	2.3
26	BD	45	TYR	2.3
29	DG	117	PRO	2.3
32	BK	120	PRO	2.3
1	AA	498	A	2.3
23	BB	91	A	2.3
23	BB	2183	A	2.3
28	BF	19	PHE	2.3
31	DJ	119	PHE	2.3
1	CA	1094	G	2.3
1	CA	1305	G	2.3
22	DA	67	G	2.3
40	DS	12	SER	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
11	CL	19	ASN	2.3
26	DD	43	ASP	2.3
28	BF	122	ASP	2.3
31	DJ	19	ASP	2.3
3	CD	159	GLU	2.3
26	BD	81	GLU	2.3
42	DU	36	GLU	2.3
1	CA	1066	C	2.3
8	CI	116	GLY	2.3
15	CP	62	GLY	2.3
23	DB	1049	C	2.3
27	DE	151	GLY	2.3
12	AM	112	ARG	2.3
13	AN	68	ARG	2.3
25	BC	220	ARG	2.3
25	BC	269	ARG	2.3
33	DL	116	VAL	2.3
36	DO	28	VAL	2.3
38	BQ	5	ARG	2.3
41	BT	6	ARG	2.3
41	DT	96	VAL	2.3
8	AI	83	THR	2.3
14	CO	69	LEU	2.3
25	DC	206	LYS	2.3
39	BR	48	LYS	2.3
31	BJ	101	ILE	2.3
33	BL	101	ILE	2.3
39	DR	41	ILE	2.3
13	AN	3	GLN	2.3
26	DD	36	GLN	2.3
29	BG	7	PRO	2.3
1	AA	1301	U	2.3
1	CA	1168	U	2.3
23	BB	2321	U	2.3
1	AA	250	A	2.3
1	AA	1101	A	2.3
1	AA	1201	A	2.3
1	CA	452	A	2.3
2	AC	12	GLY	2.3
6	AG	80	GLY	2.3
7	AH	109	VAL	2.3
8	AI	11	ARG	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
21	CU	8	ASN	2.3
23	BB	2872	A	2.3
23	DB	2108	A	2.3
25	DC	34	GLU	2.3
26	BD	165	MET	2.3
25	DC	86	ARG	2.3
30	BH	86	ASP	2.3
32	BK	18	ARG	2.3
35	DN	127	GLU	2.3
13	AN	71	GLY	2.3
30	BH	106	ALA	2.3
33	BL	90	VAL	2.3
36	DO	49	VAL	2.3
40	BS	18	ARG	2.3
41	DT	58	VAL	2.3
45	BY	1	ALA	2.3
49	B2	44	VAL	2.3
51	D4	17	VAL	2.3
51	D4	24	ARG	2.3
52	BI	62	ALA	2.3
1	CA	240	G	2.3
11	AL	115	LYS	2.3
13	AN	45	LEU	2.3
23	BB	512	G	2.3
23	BB	733	G	2.3
23	BB	784	G	2.3
23	BB	2157	G	2.3
23	DB	1099	G	2.3
27	DE	57	LYS	2.3
27	DE	99	LYS	2.3
28	DF	71	LYS	2.3
31	BJ	132	HIS	2.3
44	BX	41	HIS	2.3
52	DI	96	LYS	2.3
35	DN	98	LEU	2.3
38	BQ	89	ILE	2.3
52	BI	100	ILE	2.3
1	AA	235	C	2.3
12	AM	19	THR	2.3
23	BB	1104	C	2.3
34	BM	42	THR	2.3
26	DD	150	GLN	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
42	BU	45	GLN	2.3
30	BH	97	ARG	2.3
2	CC	62	SER	2.3
7	CH	72	GLU	2.3
16	CQ	62	GLU	2.3
20	CB	97	GLY	2.3
24	DV	15	GLY	2.3
27	BE	146	VAL	2.3
27	BE	193	VAL	2.3
25	BC	45	ASN	2.3
27	DE	95	LYS	2.3
30	BH	81	ALA	2.3
31	DJ	9	GLU	2.3
33	BL	116	VAL	2.3
42	DU	30	SER	2.3
43	DW	16	GLU	2.3
43	DW	32	ALA	2.3
48	B1	11	VAL	2.3
49	D2	45	SER	2.3
34	DM	11	LYS	2.3
35	BN	32	GLU	2.3
37	BP	43	GLU	2.3
47	D0	31	LYS	2.3
48	B1	7	LYS	2.3
48	B1	17	GLY	2.3
51	D4	34	LYS	2.3
6	CG	21	LEU	2.3
20	CB	147	LEU	2.3
23	DB	34	U	2.3
23	DB	355	U	2.3
23	DB	931	U	2.3
23	DB	1097	U	2.3
27	DE	184	ASP	2.3
33	BL	95	LEU	2.3
34	BM	124	LEU	2.3
1	AA	1004	A	2.3
23	BB	2682	A	2.3
23	DB	508	A	2.3
36	DO	87	ILE	2.3
37	BP	21	PRO	2.3
5	CF	80	PHE	2.3
8	CI	38	PHE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	CA	31	G	2.3
1	CA	201	G	2.3
6	CG	153	TYR	2.3
14	AO	61	GLN	2.3
27	DE	90	GLN	2.3
23	DB	1510	G	2.3
23	DB	1930	G	2.3
23	DB	2100	G	2.3
23	DB	2645	G	2.3
23	DB	2791	G	2.3
1	CA	183	C	2.3
23	DB	331	C	2.3
23	DB	1079	C	2.3
8	AI	56	MET	2.3
9	AJ	31	ARG	2.3
12	AM	97	ARG	2.3
21	AU	46	ARG	2.3
31	BJ	1	MET	2.3
42	BU	93	ARG	2.3
11	AL	47	ALA	2.3
18	AS	50	VAL	2.3
15	AP	30	GLY	2.3
19	AT	80	ALA	2.3
20	CB	33	ALA	2.3
27	BE	196	VAL	2.3
28	DF	30	VAL	2.3
28	DF	131	VAL	2.3
43	BW	30	VAL	2.3
43	BW	74	LYS	2.3
47	B0	36	LYS	2.3
50	B3	14	LYS	2.3
31	BJ	6	ALA	2.3
46	DZ	14	ALA	2.3
3	CD	20	LEU	2.3
20	CB	225	SER	2.3
27	DE	164	LEU	2.3
30	BH	90	LEU	2.3
39	DR	15	SER	2.3
45	DY	28	LEU	2.3
3	AD	28	ASP	2.2
6	CG	27	ASN	2.2
9	AJ	60	ASP	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
10	CK	117	HIS	2.2
15	CP	57	ILE	2.2
25	BC	196	ASN	2.2
28	DF	135	ILE	2.2
30	DH	20	ASN	2.2
48	B1	18	HIS	2.2
1	AA	5	U	2.2
23	BB	2871	U	2.2
20	CB	197	PHE	2.2
26	BD	51	THR	2.2
29	DG	7	PRO	2.2
1	AA	74	A	2.2
3	AD	203	TYR	2.2
8	CI	6	TYR	2.2
23	DB	1237	A	2.2
25	DC	61	TYR	2.2
27	DE	136	GLN	2.2
28	BF	127	TYR	2.2
29	BG	93	TYR	2.2
36	DO	116	GLN	2.2
19	AT	9	ARG	2.2
32	BK	49	ARG	2.2
36	BO	102	ARG	2.2
36	DO	13	ARG	2.2
40	DS	41	LYS	2.2
52	BI	86	LYS	2.2
39	DR	14	VAL	2.2
3	AD	23	GLY	2.2
18	AS	74	ALA	2.2
19	AT	65	LEU	2.2
26	DD	144	GLY	2.2
27	BE	12	LEU	2.2
27	DE	142	ALA	2.2
30	DH	58	LEU	2.2
36	DO	51	ALA	2.2
43	BW	21	GLY	2.2
49	B2	42	LEU	2.2
1	AA	113	G	2.2
1	AA	436	C	2.2
1	CA	281	G	2.2
1	CA	1033	G	2.2
23	BB	1053	C	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
23	BB	1870	C	2.2
8	AI	111	GLU	2.2
9	CJ	66	GLU	2.2
23	BB	2608	G	2.2
23	DB	1112	G	2.2
25	BC	184	GLU	2.2
28	DF	31	GLU	2.2
33	BL	51	GLU	2.2
3	CD	27	ILE	2.2
8	CI	64	ILE	2.2
31	BJ	40	HIS	2.2
31	DJ	130	HIS	2.2
42	DU	64	ILE	2.2
43	BW	81	ILE	2.2
47	D0	41	HIS	2.2
52	DI	34	ILE	2.2
20	CB	35	ASN	2.2
20	CB	193	ASP	2.2
33	BL	81	ASP	2.2
9	AJ	55	PRO	2.2
10	AK	88	PRO	2.2
41	BT	95	PHE	2.2
27	DE	150	THR	2.2
1	AA	965	U	2.2
1	CA	467	U	2.2
19	AT	28	ARG	2.2
5	CF	4	TYR	2.2
8	AI	63	TYR	2.2
23	BB	2139	U	2.2
30	DH	2	GLN	2.2
37	BP	20	ARG	2.2
38	BQ	54	ARG	2.2
11	CL	14	LYS	2.2
20	AB	26	MET	2.2
34	BM	62	LYS	2.2
36	DO	4	LYS	2.2
48	D1	37	LYS	2.2
52	DI	3	LYS	2.2
8	AI	18	VAL	2.2
34	DM	67	VAL	2.2
36	DO	47	VAL	2.2
37	DP	16	VAL	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
39	DR	63	VAL	2.2
46	DZ	57	VAL	2.2
1	CA	1201	A	2.2
9	AJ	61	ALA	2.2
22	DA	29	A	2.2
23	BB	310	A	2.2
23	BB	933	A	2.2
23	BB	2108	A	2.2
23	DB	482	A	2.2
26	DD	4	LEU	2.2
26	DD	75	ALA	2.2
27	BE	157	LEU	2.2
27	BE	180	LEU	2.2
28	DF	35	LEU	2.2
29	BG	4	ALA	2.2
33	BL	112	LEU	2.2
38	DQ	115	ALA	2.2
46	DZ	34	LEU	2.2
11	AL	99	GLY	2.2
15	AP	62	GLY	2.2
26	DD	44	GLY	2.2
44	BX	62	GLY	2.2
8	CI	27	ILE	2.2
13	CN	92	ILE	2.2
30	DH	143	ILE	2.2
31	DJ	81	ILE	2.2
52	DI	85	ILE	2.2
6	AG	145	GLU	2.2
44	DX	10	SER	2.2
5	CF	52	ASN	2.2
13	CN	61	ASN	2.2
18	CS	60	PHE	2.2
23	BB	1592	C	2.2
30	BH	118	PRO	2.2
42	DU	49	PRO	2.2
13	AN	52	ARG	2.2
27	BE	40	ARG	2.2
41	DT	77	ARG	2.2
1	CA	377	G	2.2
13	CN	6	LYS	2.2
23	BB	43	G	2.2
23	DB	1311	G	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
23	DB	2413	G	2.2
33	BL	121	THR	2.2
2	CC	167	TYR	2.2
7	AH	110	MET	2.2
46	BZ	18	CYS	2.2
41	BT	31	VAL	2.2
27	BE	133	LEU	2.2
29	DG	132	LEU	2.2
30	DH	12	LEU	2.2
31	BJ	109	LEU	2.2
4	CE	16	ALA	2.2
23	BB	931	U	2.2
23	DB	1058	U	2.2
31	DJ	20	ALA	2.2
33	DL	24	GLY	2.2
39	BR	100	GLY	2.2
12	AM	72	ILE	2.2
24	DV	70	ILE	2.2
1	AA	65	A	2.2
1	AA	1306	A	2.2
27	DE	152	GLU	2.2
2	CC	87	ARG	2.2
7	CH	44	PHE	2.2
12	CM	28	ARG	2.2
24	DV	21	ARG	2.2
25	DC	39	SER	2.2
27	BE	55	SER	2.2
32	BK	79	PHE	2.2
32	DK	30	ARG	2.2
33	DL	48	ARG	2.2
36	DO	33	ARG	2.2
40	DS	11	ARG	2.2
42	BU	67	SER	2.2
44	BX	29	ARG	2.2
52	DI	66	PHE	2.2
31	DJ	85	LYS	2.2
42	DU	18	LYS	2.2
5	CF	82	ASP	2.2
26	BD	200	ASP	2.2
8	CI	87	MET	2.2
26	DD	61	THR	2.2
28	DF	129	MET	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
31	DJ	5	THR	2.2
1	AA	995	C	2.2
3	CD	35	GLN	2.2
12	AM	42	VAL	2.2
27	BE	153	LEU	2.2
27	DE	115	GLN	2.2
30	BH	108	VAL	2.2
35	BN	116	VAL	2.2
38	DQ	59	LEU	2.2
50	D3	61	LEU	2.2
20	CB	82	ALA	2.2
26	DD	206	ALA	2.2
27	BE	45	ALA	2.2
37	BP	94	ALA	2.2
38	DQ	1	ALA	2.2
44	DX	32	ALA	2.2
25	DC	11	GLY	2.2
26	BD	191	GLY	2.2
33	DL	140	GLY	2.2
1	AA	428	G	2.2
1	CA	1127	G	2.2
1	CA	1190	G	2.2
23	BB	2405	G	2.2
23	DB	1450	G	2.2
26	DD	22	ILE	2.2
1	AA	407	U	2.2
23	BB	162	U	2.2
23	BB	2105	U	2.2
6	AG	9	ARG	2.2
11	AL	98	ARG	2.2
20	CB	20	ARG	2.2
29	DG	152	ARG	2.2
33	DL	143	GLU	2.2
35	BN	17	ARG	2.2
37	BP	111	GLU	2.2
49	B2	12	ARG	2.2
20	AB	142	LYS	2.2
26	BD	114	LYS	2.2
29	BG	157	LYS	2.2
33	BL	141	LYS	2.2
5	CF	42	TRP	2.2
20	AB	95	TRP	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
25	DC	10	PRO	2.2
23	BB	1508	A	2.2
23	BB	2135	A	2.2
13	CN	15	LEU	2.2
14	CO	21	THR	2.2
16	AQ	7	LEU	2.2
20	AB	129	THR	2.2
21	AU	52	VAL	2.2
26	DD	26	VAL	2.2
36	DO	115	LEU	2.2
37	BP	81	ASP	2.2
38	BQ	109	VAL	2.2
42	BU	66	VAL	2.2
25	BC	162	GLN	2.2
30	DH	81	ALA	2.1
32	BK	119	ALA	2.1
33	DL	72	ALA	2.1
41	DT	35	ALA	2.1
18	CS	67	GLY	2.1
29	BG	52	GLY	2.1
34	DM	39	GLY	2.1
3	AD	27	ILE	2.1
9	AJ	100	ILE	2.1
16	AQ	60	ILE	2.1
28	BF	153	ILE	2.1
1	CA	1031	C	2.1
23	BB	1398	C	2.1
15	AP	8	ARG	2.1
34	BM	114	ARG	2.1
32	BK	45	GLU	2.1
34	DM	115	GLU	2.1
1	AA	485	U	2.1
1	AA	531	U	2.1
1	CA	723	U	2.1
23	BB	2884	U	2.1
1	AA	69	G	2.1
1	CA	1260	G	2.1
50	D3	45	PRO	2.1
27	BE	100	MET	2.1
2	AC	153	SER	2.1
2	CC	186	SER	2.1
15	AP	44	SER	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
30	BH	37	VAL	2.1
35	BN	76	VAL	2.1
4	CE	130	THR	2.1
32	BK	104	THR	2.1
44	DX	55	THR	2.1
18	CS	11	ASP	2.1
24	BV	74	ALA	2.1
25	BC	160	TYR	2.1
27	BE	86	ALA	2.1
29	DG	12	ALA	2.1
30	DH	74	ALA	2.1
37	DP	57	ALA	2.1
38	BQ	36	GLN	2.1
38	DQ	95	ALA	2.1
40	BS	22	ASP	2.1
1	AA	98	A	2.1
1	AA	1227	A	2.1
1	CA	1493	A	2.1
23	DB	2733	A	2.1
4	CE	133	ILE	2.1
12	CM	3	ILE	2.1
26	DD	48	ILE	2.1
39	BR	59	ILE	2.1
41	BT	71	GLY	2.1
5	AF	79	ARG	2.1
30	DH	68	ARG	2.1
31	BJ	13	ARG	2.1
31	DJ	116	ARG	2.1
36	DO	9	ARG	2.1
28	BF	71	LYS	2.1
35	DN	102	PHE	2.1
26	DD	64	GLU	2.1
1	AA	1226	C	2.1
1	CA	1533	C	2.1
20	AB	28	PRO	2.1
23	DB	1052	C	2.1
40	DS	80	PRO	2.1
3	AD	8	LEU	2.1
5	CF	62	MET	2.1
52	DI	78	LEU	2.1
8	CI	110	VAL	2.1
21	AU	13	VAL	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
27	DE	96	VAL	2.1
23	BB	12	U	2.1
3	AD	204	SER	2.1
7	CH	78	SER	2.1
18	CS	24	SER	2.1
36	DO	95	SER	2.1
43	DW	80	SER	2.1
8	AI	120	ALA	2.1
15	CP	3	THR	2.1
26	DD	52	THR	2.1
32	DK	83	ALA	2.1
34	BM	7	THR	2.1
34	BM	48	ALA	2.1
39	DR	36	ALA	2.1
40	DS	44	ALA	2.1
43	DW	46	ALA	2.1
34	DM	103	TYR	2.1
35	DN	94	TYR	2.1
11	AL	5	GLN	2.1
1	AA	481	G	2.1
1	CA	725	G	2.1
1	CA	1370	G	2.1
2	AC	157	GLY	2.1
12	AM	87	GLY	2.1
14	AO	67	ASP	2.1
38	BQ	43	GLN	2.1
38	DQ	16	ILE	2.1
4	AE	53	ARG	2.1
13	AN	23	ARG	2.1
23	BB	2791	G	2.1
23	DB	287	G	2.1
29	BG	43	LYS	2.1
32	DK	105	ARG	2.1
37	BP	61	ARG	2.1
39	BR	68	ARG	2.1
50	B3	7	ARG	2.1
51	B4	2	LYS	2.1
1	AA	1000	A	2.1
1	AA	1534	A	2.1
1	CA	459	A	2.1
23	BB	2665	A	2.1
23	DB	613	A	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
23	DB	1142	A	2.1
30	BH	139	PHE	2.1
18	AS	4	LEU	2.1
28	BF	28	PRO	2.1
45	DY	58	GLU	2.1
35	BN	54	LEU	2.1
7	AH	71	VAL	2.1
20	AB	198	VAL	2.1
25	DC	219	VAL	2.1
29	DG	168	VAL	2.1
30	DH	130	VAL	2.1
1	AA	1038	C	2.1
2	CC	103	ALA	2.1
5	AF	66	ALA	2.1
23	BB	1211	C	2.1
23	BB	1726	C	2.1
23	BB	2179	C	2.1
23	BB	2467	C	2.1
23	DB	334	C	2.1
23	DB	1732	C	2.1
27	BE	8	ALA	2.1
52	DI	82	ALA	2.1
13	AN	55	SER	2.1
41	BT	22	THR	2.1
43	DW	57	THR	2.1
52	BI	20	SER	2.1
8	AI	37	TYR	2.1
11	AL	37	TYR	2.1
18	AS	55	GLN	2.1
23	BB	34	U	2.1
23	BB	2149	U	2.1
23	DB	1078	U	2.1
25	DC	255	LYS	2.1
26	BD	49	GLN	2.1
27	BE	123	LYS	2.1
27	BE	195	GLN	2.1
29	DG	43	LYS	2.1
31	BJ	27	ARG	2.1
40	DS	110	ARG	2.1
44	DX	29	ARG	2.1
46	DZ	63	ARG	2.1
52	BI	39	LYS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
52	BI	130	GLY	2.1
41	DT	59	ASN	2.1
44	BX	39	GLN	2.1
28	DF	152	ASP	2.1
1	AA	126	G	2.1
1	AA	424	G	2.1
10	CK	90	PRO	2.1
11	AL	103	CYS	2.1
23	BB	1062	G	2.1
23	BB	2186	G	2.1
23	DB	273	G	2.1
29	DG	36	LEU	2.1
34	BM	109	PRO	2.1
36	DO	83	LEU	2.1
41	DT	7	LEU	2.1
42	BU	47	PRO	2.1
44	BX	22	LEU	2.1
44	BX	37	LEU	2.1
51	B4	14	CYS	2.1
1	AA	130	A	2.1
2	AC	104	GLU	2.1
6	AG	86	VAL	2.1
11	AL	3	VAL	2.1
13	AN	33	VAL	2.1
14	CO	44	GLU	2.1
23	BB	819	A	2.1
23	BB	2883	A	2.1
23	DB	1070	A	2.1
26	DD	168	GLU	2.1
44	BX	8	GLU	2.1
25	BC	223	ALA	2.1
38	DQ	20	ALA	2.1
6	AG	69	ARG	2.1
8	CI	98	ARG	2.1
9	CJ	76	ILE	2.1
15	CP	46	LYS	2.1
24	DV	9	ARG	2.1
25	DC	155	ARG	2.1
31	BJ	95	ARG	2.1
34	DM	55	ARG	2.1
38	DQ	89	ILE	2.1
40	BS	11	ARG	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
41	DT	12	ARG	2.1
43	BW	43	LYS	2.1
43	DW	81	ILE	2.1
48	B1	49	LYS	2.1
49	D2	11	LYS	2.1
51	B4	16	ILE	2.1
6	AG	84	TYR	2.1
8	AI	8	THR	2.1
11	AL	39	THR	2.1
20	CB	19	THR	2.1
18	AS	34	SER	2.1
20	CB	212	TYR	2.1
25	BC	150	GLY	2.1
27	DE	65	THR	2.1
31	DJ	70	THR	2.1
33	BL	88	GLY	2.1
34	DM	74	THR	2.1
39	BR	57	GLY	2.1
39	BR	94	THR	2.1
46	BZ	55	GLY	2.1
46	DZ	29	GLY	2.1
25	DC	9	SER	2.1
36	BO	95	SER	2.1
37	BP	84	SER	2.1
36	BO	98	GLN	2.1
37	DP	51	ASN	2.1
46	DZ	65	ASN	2.1
1	CA	169	C	2.1
20	AB	152	ASP	2.1
23	BB	921	C	2.1
23	BB	1460	U	2.1
23	BB	2272	U	2.1
23	DB	1094	U	2.1
52	BI	120	ASP	2.1
6	AG	49	LEU	2.1
44	DX	6	LEU	2.1
52	BI	137	LEU	2.1
26	DD	104	VAL	2.1
26	DD	142	VAL	2.1
26	DD	180	VAL	2.1
44	DX	11	VAL	2.1
36	BO	60	GLU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
52	BI	36	GLU	2.1
3	AD	120	LYS	2.0
3	CD	82	LYS	2.0
20	CB	171	ALA	2.0
27	BE	106	LYS	2.0
35	BN	118	ARG	2.0
37	DP	5	LYS	2.0
38	DQ	14	LYS	2.0
1	AA	373	A	2.0
1	CA	724	G	2.0
10	AK	53	GLY	2.0
13	CN	67	GLY	2.0
23	DB	1095	A	2.0
23	DB	2311	A	2.0
23	BB	1540	G	2.0
23	BB	1869	G	2.0
23	DB	1731	G	2.0
25	DC	240	GLY	2.0
26	DD	72	GLY	2.0
2	CC	20	THR	2.0
20	AB	118	THR	2.0
30	BH	96	THR	2.0
49	D2	24	THR	2.0
14	AO	51	SER	2.0
24	BV	75	GLN	2.0
31	BJ	136	GLN	2.0
36	BO	116	GLN	2.0
43	BW	75	ASN	2.0
3	CD	17	ASP	2.0
3	CD	190	LEU	2.0
15	AP	52	LEU	2.0
31	DJ	52	ASP	2.0
34	BM	112	LEU	2.0
41	DT	32	LEU	2.0
20	AB	99	MET	2.0
1	AA	1451	U	2.0
1	CA	372	C	2.0
1	CA	1159	U	2.0
2	CC	173	PRO	2.0
11	AL	21	PRO	2.0
22	BA	49	C	2.0
22	BA	89	U	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
27	DE	120	VAL	2.0
34	BM	67	VAL	2.0
2	AC	169	GLU	2.0
3	AD	103	ARG	2.0
14	AO	25	GLU	2.0
15	AP	28	ARG	2.0
19	CT	8	LYS	2.0
20	CB	94	ARG	2.0
26	DD	81	GLU	2.0
26	DD	157	LYS	2.0
31	DJ	72	LYS	2.0
36	DO	55	GLU	2.0
37	DP	13	LYS	2.0
40	BS	88	ARG	2.0
41	BT	9	LYS	2.0
46	DZ	56	ARG	2.0
47	B0	35	GLU	2.0
52	BI	80	LYS	2.0
2	AC	195	ILE	2.0
6	CG	60	ALA	2.0
7	CH	74	ILE	2.0
12	CM	72	ILE	2.0
27	DE	8	ALA	2.0
31	DJ	42	ALA	2.0
35	BN	113	ILE	2.0
42	DU	11	ILE	2.0
43	DW	60	ALA	2.0
11	CL	70	GLY	2.0
26	DD	158	GLY	2.0
36	DO	22	GLY	2.0
6	AG	48	THR	2.0
14	CO	24	THR	2.0
17	CR	22	TYR	2.0
28	DF	7	TYR	2.0
31	DJ	16	TYR	2.0
37	BP	75	THR	2.0
8	CI	19	PHE	2.0
18	CS	9	PHE	2.0
20	AB	121	GLN	2.0
21	CU	36	PHE	2.0
51	D4	35	GLN	2.0
13	CN	31	SER	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
23	BB	1142	A	2.0
23	DB	1021	A	2.0
8	AI	97	LEU	2.0
17	CR	66	LEU	2.0
32	BK	58	LEU	2.0
40	BS	33	LEU	2.0
42	BU	97	SER	2.0
2	AC	184	ASN	2.0
29	DG	37	ASN	2.0
1	AA	104	G	2.0
1	AA	410	G	2.0
9	CJ	74	VAL	2.0
13	AN	53	ASP	2.0
18	AS	18	VAL	2.0
23	BB	1527	G	2.0
23	BB	2152	G	2.0
23	BB	2732	G	2.0
23	BB	2867	G	2.0
23	DB	549	G	2.0
28	BF	11	VAL	2.0
40	DS	22	ASP	2.0
52	DI	63	ASP	2.0
3	CD	185	PRO	2.0
15	AP	41	PRO	2.0
10	AK	23	HIS	2.0
19	CT	74	HIS	2.0
27	BE	21	ARG	2.0
37	DP	76	HIS	2.0
38	BQ	21	LYS	2.0
47	D0	15	ARG	2.0
2	AC	179	ALA	2.0
13	AN	9	GLU	2.0
15	AP	72	ALA	2.0
28	DF	44	ALA	2.0
29	DG	80	GLU	2.0
31	BJ	104	ALA	2.0
34	DM	121	ALA	2.0
38	DQ	79	ILE	2.0
43	DW	69	GLU	2.0
52	BI	82	ALA	2.0
23	DB	1730	C	2.0
33	BL	44	GLY	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
37	BP	44	GLY	2.0
37	DP	53	GLY	2.0

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

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

5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	AA	1636	1/1	0.55	0.37	127,127,127,127	0
53	MG	DB	3059	1/1	0.61	0.14	127,127,127,127	0
53	MG	AA	1649	1/1	0.67	0.16	114,114,114,114	0
53	MG	CA	1623	1/1	0.68	0.14	151,151,151,151	0
53	MG	AA	1612	1/1	0.71	0.16	104,104,104,104	0
53	MG	AA	1629	1/1	0.72	0.18	138,138,138,138	0
53	MG	AA	1622	1/1	0.78	0.14	116,116,116,116	0
53	MG	BB	3067	1/1	0.78	0.15	78,78,78,78	0
53	MG	AA	1644	1/1	0.81	0.12	96,96,96,96	0
53	MG	AA	1619	1/1	0.82	0.13	100,100,100,100	0
53	MG	DB	3082	1/1	0.83	0.15	73,73,73,73	0
53	MG	AA	1638	1/1	0.84	0.16	98,98,98,98	0
53	MG	AA	1658	1/1	0.84	0.16	167,167,167,167	0
53	MG	AA	1623	1/1	0.85	0.23	32,32,32,32	1
53	MG	AP	101	1/1	0.85	0.19	53,53,53,53	1
53	MG	CA	1616	1/1	0.86	0.18	68,68,68,68	0
53	MG	BB	3042	1/1	0.88	0.07	95,95,95,95	0
53	MG	CA	1615	1/1	0.88	0.11	101,101,101,101	0
53	MG	BB	3081	1/1	0.89	0.10	46,46,46,46	0
53	MG	BB	3082	1/1	0.89	0.12	19,19,19,19	0
53	MG	DB	3034	1/1	0.89	0.14	66,66,66,66	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	BB	3090	1/1	0.89	0.08	74,74,74,74	0
53	MG	AA	1608	1/1	0.89	0.12	121,121,121,121	0
53	MG	BB	3110	1/1	0.90	0.15	60,60,60,60	0
53	MG	BB	3063	1/1	0.90	0.11	27,27,27,27	0
53	MG	CA	1628	1/1	0.90	0.13	55,55,55,55	1
53	MG	AA	1655	1/1	0.91	0.14	75,75,75,75	0
53	MG	CA	1621	1/1	0.91	0.15	113,113,113,113	0
53	MG	DB	3013	1/1	0.91	0.12	34,34,34,34	0
53	MG	BB	3060	1/1	0.92	0.08	69,69,69,69	0
53	MG	BB	3021	1/1	0.92	0.12	55,55,55,55	0
53	MG	AA	1614	1/1	0.92	0.09	62,62,62,62	0
53	MG	DB	3065	1/1	0.92	0.26	47,47,47,47	1
53	MG	CA	1632	1/1	0.92	0.09	61,61,61,61	0
53	MG	CA	1639	1/1	0.93	0.07	117,117,117,117	0
53	MG	AA	1659	1/1	0.93	0.07	105,105,105,105	0
53	MG	DB	3024	1/1	0.93	0.11	36,36,36,36	0
53	MG	BB	3088	1/1	0.93	0.13	34,34,34,34	0
53	MG	BB	3026	1/1	0.93	0.08	5,5,5,5	0
53	MG	DB	3060	1/1	0.93	0.08	77,77,77,77	0
53	MG	BB	3033	1/1	0.93	0.10	93,93,93,93	0
53	MG	AA	1641	1/1	0.93	0.09	49,49,49,49	0
53	MG	DB	3091	1/1	0.93	0.08	96,96,96,96	0
53	MG	DB	3104	1/1	0.93	0.07	50,50,50,50	0
53	MG	CA	1634	1/1	0.94	0.10	61,61,61,61	0
53	MG	AA	1657	1/1	0.94	0.09	81,81,81,81	0
53	MG	CA	1648	1/1	0.94	0.14	56,56,56,56	0
53	MG	CA	1660	1/1	0.94	0.09	65,65,65,65	0
53	MG	BB	3094	1/1	0.94	0.06	35,35,35,35	0
53	MG	AA	1654	1/1	0.94	0.10	59,59,59,59	0
53	MG	DB	3103	1/1	0.94	0.09	50,50,50,50	0
53	MG	DB	3030	1/1	0.94	0.09	23,23,23,23	0
53	MG	AA	1637	1/1	0.95	0.08	81,81,81,81	0
53	MG	BB	3074	1/1	0.95	0.09	13,13,13,13	0
53	MG	BB	3093	1/1	0.95	0.20	5,5,5,5	1
53	MG	CA	1627	1/1	0.95	0.13	29,29,29,29	1
53	MG	BB	3079	1/1	0.95	0.11	38,38,38,38	0
53	MG	BB	3096	1/1	0.95	0.07	43,43,43,43	0
53	MG	AA	1639	1/1	0.95	0.06	47,47,47,47	0
53	MG	CA	1637	1/1	0.95	0.10	68,68,68,68	0
53	MG	CA	1608	1/1	0.95	0.12	110,110,110,110	0
53	MG	BB	3034	1/1	0.95	0.08	25,25,25,25	0
53	MG	CA	1649	1/1	0.95	0.14	88,88,88,88	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	CA	1650	1/1	0.95	0.09	82,82,82,82	0
53	MG	BB	3046	1/1	0.96	0.07	51,51,51,51	0
53	MG	BB	3047	1/1	0.96	0.06	114,114,114,114	0
53	MG	CA	1645	1/1	0.96	0.12	82,82,82,82	0
53	MG	AA	1617	1/1	0.96	0.07	78,78,78,78	0
53	MG	BB	3100	1/1	0.96	0.17	11,11,11,11	1
53	MG	BB	3010	1/1	0.96	0.09	39,39,39,39	0
53	MG	BB	3017	1/1	0.96	0.08	72,72,72,72	0
53	MG	CA	1611	1/1	0.96	0.07	71,71,71,71	0
53	MG	CA	1613	1/1	0.96	0.08	78,78,78,78	0
53	MG	AA	1624	1/1	0.96	0.15	79,79,79,79	0
53	MG	BB	3077	1/1	0.96	0.09	44,44,44,44	0
53	MG	DB	3058	1/1	0.96	0.10	30,30,30,30	1
53	MG	BB	3078	1/1	0.96	0.18	25,25,25,25	0
53	MG	AA	1605	1/1	0.96	0.07	48,48,48,48	0
53	MG	CA	1624	1/1	0.96	0.09	48,48,48,48	0
53	MG	BB	3028	1/1	0.96	0.10	40,40,40,40	0
53	MG	AA	1635	1/1	0.96	0.08	85,85,85,85	0
53	MG	AA	1602	1/1	0.96	0.05	62,62,62,62	0
53	MG	AA	1648	1/1	0.96	0.06	94,94,94,94	0
53	MG	AA	1632	1/1	0.97	0.05	53,53,53,53	0
53	MG	BB	3051	1/1	0.97	0.06	71,71,71,71	0
53	MG	CA	1636	1/1	0.97	0.09	51,51,51,51	0
53	MG	AA	1633	1/1	0.97	0.05	75,75,75,75	0
53	MG	AA	1634	1/1	0.97	0.09	85,85,85,85	0
53	MG	CA	1641	1/1	0.97	0.14	92,92,92,92	0
53	MG	CA	1643	1/1	0.97	0.06	41,41,41,41	0
53	MG	BB	3098	1/1	0.97	0.08	45,45,45,45	0
53	MG	BB	3065	1/1	0.97	0.08	47,47,47,47	0
53	MG	BB	3105	1/1	0.97	0.16	64,64,64,64	0
53	MG	AA	1604	1/1	0.97	0.08	45,45,45,45	0
53	MG	CA	1657	1/1	0.97	0.06	37,37,37,37	0
53	MG	CA	1603	1/1	0.97	0.11	69,69,69,69	0
53	MG	CA	1662	1/1	0.97	0.09	26,26,26,26	0
53	MG	CA	1606	1/1	0.97	0.06	74,74,74,74	0
53	MG	DB	3015	1/1	0.97	0.06	49,49,49,49	0
53	MG	BB	3030	1/1	0.97	0.05	53,53,53,53	0
53	MG	BB	3075	1/1	0.97	0.11	31,31,31,31	0
53	MG	AA	1611	1/1	0.97	0.07	40,40,40,40	0
53	MG	DB	3050	1/1	0.97	0.08	74,74,74,74	0
53	MG	DB	3051	1/1	0.97	0.08	53,53,53,53	0
53	MG	DB	3052	1/1	0.97	0.17	60,60,60,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	DB	3053	1/1	0.97	0.15	27,27,27,27	0
53	MG	AA	1631	1/1	0.97	0.10	61,61,61,61	0
53	MG	BB	3041	1/1	0.97	0.05	30,30,30,30	0
53	MG	BB	3007	1/1	0.97	0.08	28,28,28,28	0
53	MG	DB	3061	1/1	0.97	0.04	78,78,78,78	0
53	MG	BB	3043	1/1	0.97	0.09	75,75,75,75	0
53	MG	DB	3077	1/1	0.97	0.08	57,57,57,57	0
53	MG	BB	3087	1/1	0.97	0.10	45,45,45,45	0
53	MG	DB	3083	1/1	0.97	0.14	27,27,27,27	0
53	MG	DB	3088	1/1	0.97	0.09	35,35,35,35	0
53	MG	DB	3089	1/1	0.97	0.05	65,65,65,65	0
53	MG	CA	1626	1/1	0.97	0.06	73,73,73,73	0
53	MG	DB	3095	1/1	0.97	0.11	55,55,55,55	0
53	MG	AA	1653	1/1	0.97	0.07	65,65,65,65	0
53	MG	BB	3089	1/1	0.97	0.07	45,45,45,45	0
53	MG	DB	3110	1/1	0.97	0.11	54,54,54,54	0
53	MG	AA	1606	1/1	0.98	0.04	59,59,59,59	0
53	MG	AA	1650	1/1	0.98	0.07	72,72,72,72	0
53	MG	CA	1635	1/1	0.98	0.05	20,20,20,20	0
53	MG	AA	1651	1/1	0.98	0.06	84,84,84,84	0
53	MG	AA	1625	1/1	0.98	0.06	5,5,5,5	1
53	MG	BB	3039	1/1	0.98	0.11	45,45,45,45	0
53	MG	AA	1626	1/1	0.98	0.07	35,35,35,35	0
53	MG	CA	1642	1/1	0.98	0.06	45,45,45,45	0
53	MG	BB	3091	1/1	0.98	0.08	19,19,19,19	0
53	MG	AA	1627	1/1	0.98	0.10	72,72,72,72	0
53	MG	AA	1656	1/1	0.98	0.16	66,66,66,66	0
53	MG	AA	1628	1/1	0.98	0.06	26,26,26,26	0
53	MG	BB	3097	1/1	0.98	0.09	74,74,74,74	0
53	MG	CA	1652	1/1	0.98	0.08	44,44,44,44	0
53	MG	AA	1607	1/1	0.98	0.06	27,27,27,27	0
53	MG	CA	1659	1/1	0.98	0.17	48,48,48,48	0
53	MG	BB	3099	1/1	0.98	0.05	30,30,30,30	0
53	MG	CA	1661	1/1	0.98	0.04	62,62,62,62	0
53	MG	BB	3049	1/1	0.98	0.08	11,11,11,11	0
53	MG	DB	3001	1/1	0.98	0.08	7,7,7,7	0
53	MG	DB	3002	1/1	0.98	0.06	37,37,37,37	0
53	MG	BB	3101	1/1	0.98	0.07	12,12,12,12	0
53	MG	AA	1620	1/1	0.98	0.09	62,62,62,62	0
53	MG	DB	3016	1/1	0.98	0.05	23,23,23,23	0
53	MG	DB	3020	1/1	0.98	0.07	20,20,20,20	0
53	MG	BB	3107	1/1	0.98	0.07	27,27,27,27	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	DB	3027	1/1	0.98	0.08	10,10,10,10	0
53	MG	DB	3029	1/1	0.98	0.17	41,41,41,41	0
53	MG	BB	3109	1/1	0.98	0.13	15,15,15,15	0
53	MG	BB	3052	1/1	0.98	0.10	19,19,19,19	0
53	MG	DB	3041	1/1	0.98	0.06	18,18,18,18	0
53	MG	DB	3045	1/1	0.98	0.04	61,61,61,61	0
53	MG	DB	3047	1/1	0.98	0.07	17,17,17,17	0
53	MG	BB	3054	1/1	0.98	0.06	72,72,72,72	0
53	MG	AA	1642	1/1	0.98	0.05	70,70,70,70	0
53	MG	AA	1643	1/1	0.98	0.05	73,73,73,73	0
53	MG	CA	1609	1/1	0.98	0.12	45,45,45,45	0
53	MG	DB	3057	1/1	0.98	0.06	28,28,28,28	0
53	MG	BB	3009	1/1	0.98	0.07	35,35,35,35	0
53	MG	AA	1603	1/1	0.98	0.05	43,43,43,43	0
53	MG	CA	1614	1/1	0.98	0.08	47,47,47,47	0
53	MG	BB	3071	1/1	0.98	0.05	24,24,24,24	0
53	MG	DB	3062	1/1	0.98	0.08	43,43,43,43	0
53	MG	BB	3072	1/1	0.98	0.06	24,24,24,24	0
53	MG	DB	3067	1/1	0.98	0.04	17,17,17,17	0
53	MG	DB	3071	1/1	0.98	0.07	39,39,39,39	0
53	MG	DB	3076	1/1	0.98	0.05	17,17,17,17	0
53	MG	BB	3013	1/1	0.98	0.07	31,31,31,31	0
53	MG	CA	1622	1/1	0.98	0.07	67,67,67,67	0
53	MG	AA	1645	1/1	0.98	0.10	27,27,27,27	0
53	MG	AA	1646	1/1	0.98	0.13	60,60,60,60	0
53	MG	CA	1625	1/1	0.98	0.08	26,26,26,26	0
53	MG	AA	1615	1/1	0.98	0.15	43,43,43,43	0
53	MG	DB	3094	1/1	0.98	0.20	5,5,5,5	1
53	MG	BB	3027	1/1	0.98	0.11	23,23,23,23	0
53	MG	DB	3102	1/1	0.98	0.05	26,26,26,26	0
53	MG	BB	3080	1/1	0.98	0.07	31,31,31,31	0
53	MG	CA	1630	1/1	0.98	0.10	5,5,5,5	1
53	MG	DB	3107	1/1	0.98	0.06	19,19,19,19	0
53	MG	CA	1631	1/1	0.98	0.07	36,36,36,36	0
53	MG	DN	201	1/1	0.98	0.12	49,49,49,49	0
53	MG	AA	1601	1/1	0.99	0.05	26,26,26,26	0
53	MG	CA	1646	1/1	0.99	0.04	42,42,42,42	0
53	MG	CA	1647	1/1	0.99	0.05	32,32,32,32	0
53	MG	BB	3095	1/1	0.99	0.03	34,34,34,34	0
53	MG	BB	3018	1/1	0.99	0.04	27,27,27,27	0
53	MG	BB	3048	1/1	0.99	0.04	20,20,20,20	0
53	MG	CA	1651	1/1	0.99	0.02	14,14,14,14	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	BB	3019	1/1	0.99	0.09	27,27,27,27	0
53	MG	CA	1653	1/1	0.99	0.17	45,45,45,45	0
53	MG	CA	1654	1/1	0.99	0.04	40,40,40,40	0
53	MG	CA	1655	1/1	0.99	0.10	48,48,48,48	0
53	MG	CA	1656	1/1	0.99	0.10	48,48,48,48	0
53	MG	BB	3050	1/1	0.99	0.05	35,35,35,35	0
53	MG	CA	1658	1/1	0.99	0.10	38,38,38,38	0
53	MG	AA	1640	1/1	0.99	0.09	44,44,44,44	0
53	MG	BB	3022	1/1	0.99	0.03	38,38,38,38	0
53	MG	BB	3102	1/1	0.99	0.04	19,19,19,19	0
53	MG	BB	3104	1/1	0.99	0.04	18,18,18,18	0
53	MG	BB	3024	1/1	0.99	0.03	22,22,22,22	0
53	MG	BB	3106	1/1	0.99	0.06	46,46,46,46	0
53	MG	DB	3003	1/1	0.99	0.04	14,14,14,14	0
53	MG	DB	3004	1/1	0.99	0.07	19,19,19,19	0
53	MG	DB	3007	1/1	0.99	0.04	12,12,12,12	0
53	MG	DB	3008	1/1	0.99	0.07	24,24,24,24	0
53	MG	BB	3055	1/1	0.99	0.06	27,27,27,27	0
53	MG	DB	3014	1/1	0.99	0.05	5,5,5,5	0
53	MG	BB	3108	1/1	0.99	0.06	19,19,19,19	0
53	MG	BB	3057	1/1	0.99	0.14	27,27,27,27	0
53	MG	DB	3018	1/1	0.99	0.04	29,29,29,29	0
53	MG	BB	3058	1/1	0.99	0.04	28,28,28,28	0
53	MG	DB	3022	1/1	0.99	0.05	15,15,15,15	0
53	MG	CA	1602	1/1	0.99	0.11	32,32,32,32	0
53	MG	DB	3025	1/1	0.99	0.06	21,21,21,21	0
53	MG	DB	3026	1/1	0.99	0.12	18,18,18,18	0
53	MG	BB	3059	1/1	0.99	0.03	10,10,10,10	0
53	MG	DB	3028	1/1	0.99	0.05	28,28,28,28	0
53	MG	BB	3025	1/1	0.99	0.07	53,53,53,53	0
53	MG	CA	1607	1/1	0.99	0.05	18,18,18,18	0
53	MG	DB	3031	1/1	0.99	0.05	18,18,18,18	0
53	MG	DB	3032	1/1	0.99	0.04	46,46,46,46	0
53	MG	BB	3061	1/1	0.99	0.06	42,42,42,42	0
53	MG	DB	3035	1/1	0.99	0.11	30,30,30,30	0
53	MG	DB	3036	1/1	0.99	0.03	16,16,16,16	0
53	MG	DB	3037	1/1	0.99	0.04	13,13,13,13	0
53	MG	DB	3040	1/1	0.99	0.06	5,5,5,5	0
53	MG	AA	1610	1/1	0.99	0.05	34,34,34,34	0
53	MG	DB	3042	1/1	0.99	0.04	27,27,27,27	0
53	MG	DB	3043	1/1	0.99	0.07	9,9,9,9	0
53	MG	BB	3064	1/1	0.99	0.07	39,39,39,39	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	DB	3046	1/1	0.99	0.04	33,33,33,33	0
53	MG	CA	1612	1/1	0.99	0.07	29,29,29,29	0
53	MG	AA	1621	1/1	0.99	0.05	23,23,23,23	0
53	MG	BB	3066	1/1	0.99	0.05	59,59,59,59	0
53	MG	BB	3005	1/1	0.99	0.07	5,5,5,5	0
53	MG	BB	3068	1/1	0.99	0.04	24,24,24,24	0
53	MG	DB	3054	1/1	0.99	0.06	15,15,15,15	0
53	MG	DB	3055	1/1	0.99	0.03	19,19,19,19	0
53	MG	CA	1620	1/1	0.99	0.03	35,35,35,35	0
53	MG	BB	3029	1/1	0.99	0.06	13,13,13,13	0
53	MG	AA	1616	1/1	0.99	0.04	46,46,46,46	0
53	MG	BB	3073	1/1	0.99	0.03	28,28,28,28	0
53	MG	BB	3031	1/1	0.99	0.17	45,45,45,45	0
53	MG	BB	3032	1/1	0.99	0.07	9,9,9,9	0
53	MG	BB	3008	1/1	0.99	0.04	58,58,58,58	0
53	MG	AA	1613	1/1	0.99	0.03	42,42,42,42	0
53	MG	DB	3068	1/1	0.99	0.06	14,14,14,14	0
53	MG	DB	3069	1/1	0.99	0.04	44,44,44,44	0
53	MG	DB	3070	1/1	0.99	0.04	46,46,46,46	0
53	MG	BB	3035	1/1	0.99	0.04	12,12,12,12	0
53	MG	DB	3072	1/1	0.99	0.04	30,30,30,30	0
53	MG	DB	3073	1/1	0.99	0.03	16,16,16,16	0
53	MG	CA	1629	1/1	0.99	0.05	45,45,45,45	0
53	MG	BB	3036	1/1	0.99	0.07	37,37,37,37	0
53	MG	DB	3078	1/1	0.99	0.03	18,18,18,18	0
53	MG	BB	3037	1/1	0.99	0.03	24,24,24,24	0
53	MG	BB	3038	1/1	0.99	0.03	58,58,58,58	0
53	MG	DB	3086	1/1	0.99	0.09	69,69,69,69	0
53	MG	DB	3087	1/1	0.99	0.03	6,6,6,6	0
53	MG	CA	1633	1/1	0.99	0.05	47,47,47,47	0
53	MG	BB	3083	1/1	0.99	0.04	20,20,20,20	0
53	MG	BB	3086	1/1	0.99	0.08	37,37,37,37	0
53	MG	AA	1630	1/1	0.99	0.04	30,30,30,30	0
53	MG	BB	3040	1/1	0.99	0.05	21,21,21,21	0
53	MG	DB	3096	1/1	0.99	0.04	20,20,20,20	0
53	MG	DB	3098	1/1	0.99	0.05	18,18,18,18	0
53	MG	DB	3099	1/1	0.99	0.04	9,9,9,9	0
53	MG	CA	1638	1/1	0.99	0.05	37,37,37,37	0
53	MG	BB	3012	1/1	0.99	0.05	41,41,41,41	0
53	MG	AA	1618	1/1	0.99	0.04	46,46,46,46	0
53	MG	DB	3105	1/1	0.99	0.06	23,23,23,23	0
53	MG	DB	3106	1/1	0.99	0.06	21,21,21,21	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	BB	3016	1/1	0.99	0.10	15,15,15,15	0
53	MG	DB	3109	1/1	0.99	0.04	24,24,24,24	0
53	MG	BB	3045	1/1	0.99	0.07	31,31,31,31	0
53	MG	CA	1644	1/1	0.99	0.04	29,29,29,29	0
53	MG	BB	3085	1/1	1.00	0.02	22,22,22,22	0
53	MG	BB	3020	1/1	1.00	0.02	23,23,23,23	0
53	MG	DB	3048	1/1	1.00	0.07	20,20,20,20	0
53	MG	DB	3049	1/1	1.00	0.02	5,5,5,5	0
53	MG	CA	1601	1/1	1.00	0.02	5,5,5,5	0
53	MG	BB	3001	1/1	1.00	0.03	10,10,10,10	0
53	MG	BB	3002	1/1	1.00	0.03	10,10,10,10	0
53	MG	DB	3005	1/1	1.00	0.02	9,9,9,9	0
53	MG	DB	3006	1/1	1.00	0.02	5,5,5,5	0
53	MG	CA	1604	1/1	1.00	0.04	18,18,18,18	0
53	MG	DB	3056	1/1	1.00	0.01	11,11,11,11	0
53	MG	CA	1605	1/1	1.00	0.03	18,18,18,18	0
53	MG	DB	3009	1/1	1.00	0.03	7,7,7,7	0
53	MG	DB	3010	1/1	1.00	0.02	12,12,12,12	0
53	MG	DB	3011	1/1	1.00	0.02	8,8,8,8	0
53	MG	DB	3012	1/1	1.00	0.05	6,6,6,6	0
53	MG	BB	3023	1/1	1.00	0.02	22,22,22,22	0
53	MG	DB	3063	1/1	1.00	0.09	13,13,13,13	0
53	MG	DB	3064	1/1	1.00	0.06	28,28,28,28	0
53	MG	BB	3011	1/1	1.00	0.06	7,7,7,7	0
53	MG	DB	3066	1/1	1.00	0.05	5,5,5,5	0
53	MG	BB	3069	1/1	1.00	0.03	9,9,9,9	0
53	MG	CA	1640	1/1	1.00	0.02	11,11,11,11	0
53	MG	DB	3017	1/1	1.00	0.03	5,5,5,5	0
53	MG	BB	3092	1/1	1.00	0.02	11,11,11,11	0
53	MG	DB	3019	1/1	1.00	0.06	5,5,5,5	0
53	MG	CA	1610	1/1	1.00	0.02	34,34,34,34	0
53	MG	DB	3021	1/1	1.00	0.03	16,16,16,16	0
53	MG	DB	3074	1/1	1.00	0.03	25,25,25,25	0
53	MG	DB	3075	1/1	1.00	0.05	5,5,5,5	0
53	MG	BB	3070	1/1	1.00	0.02	32,32,32,32	0
53	MG	DB	3023	1/1	1.00	0.03	34,34,34,34	0
53	MG	BB	3003	1/1	1.00	0.02	13,13,13,13	0
53	MG	DB	3079	1/1	1.00	0.02	5,5,5,5	0
53	MG	DB	3080	1/1	1.00	0.03	12,12,12,12	0
53	MG	DB	3081	1/1	1.00	0.04	25,25,25,25	0
53	MG	BB	3053	1/1	1.00	0.02	6,6,6,6	0
53	MG	BB	3004	1/1	1.00	0.04	21,21,21,21	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	DB	3084	1/1	1.00	0.02	8,8,8,8	0
53	MG	DB	3085	1/1	1.00	0.03	17,17,17,17	0
53	MG	BB	3014	1/1	1.00	0.03	29,29,29,29	0
53	MG	BB	3056	1/1	1.00	0.12	19,19,19,19	0
53	MG	CA	1617	1/1	1.00	0.02	9,9,9,9	0
53	MG	CA	1618	1/1	1.00	0.02	5,5,5,5	0
53	MG	DB	3090	1/1	1.00	0.05	28,28,28,28	0
53	MG	CA	1619	1/1	1.00	0.09	26,26,26,26	0
53	MG	DB	3092	1/1	1.00	0.02	23,23,23,23	0
53	MG	DB	3093	1/1	1.00	0.06	10,10,10,10	0
53	MG	BB	3076	1/1	1.00	0.03	24,24,24,24	0
53	MG	DB	3033	1/1	1.00	0.04	11,11,11,11	0
53	MG	BB	3015	1/1	1.00	0.02	24,24,24,24	0
53	MG	DB	3097	1/1	1.00	0.06	15,15,15,15	0
53	MG	AA	1652	1/1	1.00	0.04	25,25,25,25	0
53	MG	BB	3006	1/1	1.00	0.02	10,10,10,10	0
53	MG	DB	3100	1/1	1.00	0.04	11,11,11,11	0
53	MG	DB	3101	1/1	1.00	0.04	27,27,27,27	0
53	MG	BB	3103	1/1	1.00	0.03	7,7,7,7	0
53	MG	DB	3038	1/1	1.00	0.03	16,16,16,16	0
53	MG	DB	3039	1/1	1.00	0.03	19,19,19,19	0
53	MG	BB	3044	1/1	1.00	0.04	32,32,32,32	0
53	MG	AA	1609	1/1	1.00	0.05	8,8,8,8	0
53	MG	BB	3062	1/1	1.00	0.03	22,22,22,22	0
53	MG	DB	3108	1/1	1.00	0.03	5,5,5,5	0
53	MG	AA	1647	1/1	1.00	0.02	23,23,23,23	0
53	MG	DB	3044	1/1	1.00	0.04	7,7,7,7	0
53	MG	BB	3084	1/1	1.00	0.05	5,5,5,5	0

5.5 Other polymers ⓘ

There are no such residues in this entry.