



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 30, 2026 – 12:09 PM UTC

PDB ID : 4U24 / pdb_00004u24
Title : Crystal structure of the E. coli ribosome bound to dalbavancin.
Authors : Noeske, J.; Huang, J.; Olivier, N.B.; Giacobbe, R.A.; Zambrowski, M.; Cate, J.H.D.
Deposited on : 2014-07-16
Resolution : 2.90 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**
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
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) : 2.49

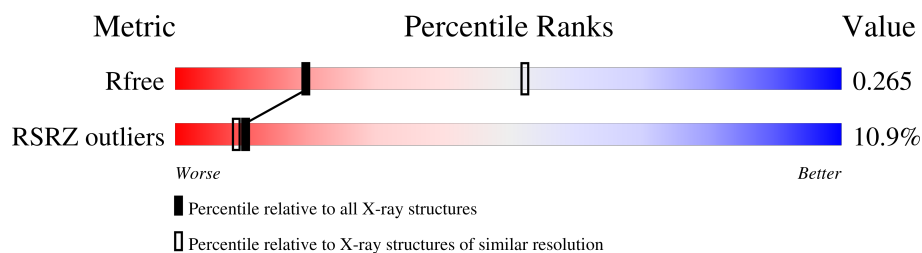
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	180053	2481 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	DA	3058	-	-	-	X
54	MG	DA	3061	-	-	-	X
54	MG	DA	3133	-	-	-	X

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 288276 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 rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1538	Total	C	N	O	P	0	0	0
			32995	14716	6050	10691	1538			
1	CA	1539	Total	C	N	O	P	0	0	0
			33015	14725	6052	10699	1539			

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	218	Total	C	N	O	S	0	0	0
			1705	1081	305	312	7			
2	CB	218	Total	C	N	O	S	0	0	0
			1705	1081	305	312	7			

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	206	Total	C	N	O	S	0	0	0
			1625	1028	305	289	3			
3	CC	206	Total	C	N	O	S	0	0	0
			1625	1028	305	289	3			

- Molecule 4 is a protein called 30S ribosomal protein S4.

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

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	150	Total	C	N	O	S	0	0	0
			1106	687	211	202	6			
5	CE	150	Total	C	N	O	S	0	0	0
			1106	687	211	202	6			

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	100	Total	C	N	O	S	0	0	0
			818	515	148	149	6			
6	CF	100	Total	C	N	O	S	0	0	0
			818	515	148	149	6			

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	151	Total	C	N	O	S	0	0	0
			1182	735	227	216	4			
7	CG	151	Total	C	N	O	S	0	0	0
			1182	735	227	216	4			

- Molecule 8 is a protein called 30S ribosomal protein S8.

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

- Molecule 9 is a protein called 30S ribosomal protein S9.

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

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	98	Total	C	N	O	S	0	0	0
			787	493	150	143	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	CJ	98	Total	C	N	O	S	0	0	0
			787	493	150	143	1			

- Molecule 11 is a protein called 30S ribosomal protein S11.

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

- Molecule 12 is a protein called 30S ribosomal protein S12.

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

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	114	Total	C	N	O	S	0	0	0
			884	546	178	157	3			
13	CM	114	Total	C	N	O	S	0	0	0
			884	546	178	157	3			

- Molecule 14 is a protein called 30S ribosomal protein S14.

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

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AO	88	Total	C	N	O	S	0	0	0
			710	437	143	129	1			
15	CO	88	Total	C	N	O	S	0	0	0
			710	437	143	129	1			

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			
16	CP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	80	Total	C	N	O	S	0	0	0
			649	411	121	114	3			
17	CQ	80	Total	C	N	O	S	0	0	0
			649	411	121	114	3			

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AR	55	Total	C	N	O	0	0	0
			456	288	86	82			
18	CR	55	Total	C	N	O	0	0	0
			456	288	86	82			

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	79	Total	C	N	O	S	0	0	0
			638	408	120	108	2			
19	CS	79	Total	C	N	O	S	0	0	0
			638	408	120	108	2			

- Molecule 20 is a protein called 30S ribosomal protein S20.

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

- 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
			426	265	86	74	1			
21	CU	51	Total	C	N	O	S	0	0	0
			426	265	86	74	1			

- Molecule 22 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	BA	2897	Total	C	N	O	P	0	0	0
			62195	27745	11446	20107	2897			
22	DA	2897	Total	C	N	O	P	0	0	0
			62195	27745	11446	20107	2897			

- Molecule 23 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	BB	119	Total	C	N	O	P	0	0	0
			2549	1135	466	829	119			
23	DB	118	Total	C	N	O	P	0	0	0
			2529	1126	464	821	118			

- Molecule 24 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	BC	271	Total	C	N	O	S	0	0	0
			2083	1288	423	365	7			
24	DC	271	Total	C	N	O	S	0	0	0
			2083	1288	423	365	7			

- Molecule 25 is a protein called 50S ribosomal protein L3.

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

- Molecule 26 is a protein called 50S ribosomal protein L4.

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

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

- Molecule 27 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BF	177	Total	C	N	O	S	0	0	0
			1411	899	249	257	6			
27	DF	177	Total	C	N	O	S	0	0	0
			1411	899	249	257	6			

- Molecule 28 is a protein called 50S ribosomal protein L6.

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

- Molecule 29 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BH	149	Total	C	N	O	S	0	0	0
			1110	699	197	213	1			
29	DH	149	Total	C	N	O	S	0	0	0
			1110	699	197	213	1			

- Molecule 30 is a protein called 50S ribosomal protein L11.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BJ	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			
31	DJ	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BK	122	Total	C	N	O	S	0	0	0
			939	587	180	166	6			
32	DK	122	Total	C	N	O	S	0	0	0
			939	587	180	166	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BL	143	Total	C	N	O	S	0	0	0
			1045	649	206	189	1			
33	DL	143	Total	C	N	O	S	0	0	0
			1045	649	206	189	1			

- 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	120	Total	C	N	O	S	0	0	0
			961	593	196	167	5			
35	DN	120	Total	C	N	O	S	0	0	0
			961	593	196	167	5			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
36	BO	116	Total	C	N	O	0	0	0
			892	552	178	162			
36	DO	116	Total	C	N	O	0	0	0
			892	552	178	162			

- 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	93	Total	C	N	O	S	0	0	0
			739	466	139	132	2			
41	DT	93	Total	C	N	O	S	0	0	0
			739	466	139	132	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
			780	492	146	142				

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
42	DU	102	Total	C	N	O	0	0	0
			780	492	146	142			

- Molecule 43 is a protein called 50S ribosomal protein L25.

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

- Molecule 44 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BW	76	Total	C	N	O	S	0	0	0
			580	359	117	103	1			
44	DW	75	Total	C	N	O	S	0	0	0
			569	353	113	102	1			

- Molecule 45 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BX	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			
45	DX	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			

- Molecule 46 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BY	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			
46	DY	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			

- Molecule 47 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BZ	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			
47	DZ	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			

- Molecule 48 is a protein called 50S ribosomal protein L32.

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

- Molecule 49 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
49	B1	50	Total	C	N	O	0	0	0
			410	263	75	72			
49	D1	50	Total	C	N	O	0	0	0
			410	263	75	72			

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

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

- Molecule 51 is a protein called 50S ribosomal protein L35.

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

- Molecule 52 is a protein called 50S ribosomal protein L36.

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

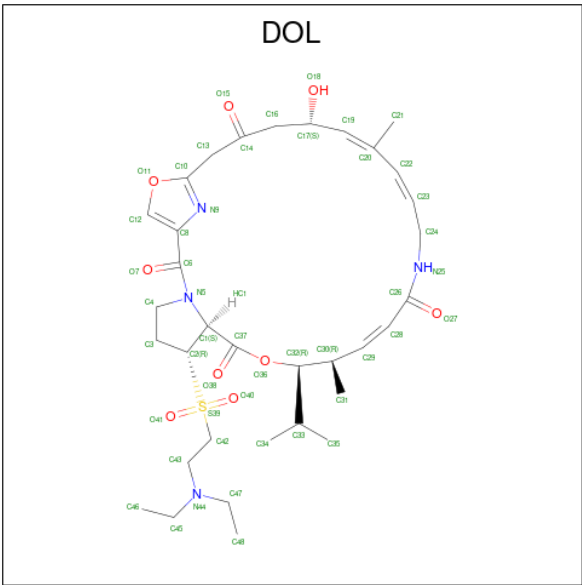
- Molecule 53 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
53	B5	191	Total	C	N	O	0	0	1
			1142	691	221	230			

- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	AA	70	Total	Mg	0	0
			70	70		
54	AM	1	Total	Mg	0	0
			1	1		
54	AN	1	Total	Mg	0	0
			1	1		
54	BA	194	Total	Mg	0	0
			194	194		
54	BB	4	Total	Mg	0	0
			4	4		
54	BQ	1	Total	Mg	0	0
			1	1		
54	CA	56	Total	Mg	0	0
			56	56		
54	DA	164	Total	Mg	0	0
			164	164		
54	DB	3	Total	Mg	0	0
			3	3		
54	DL	1	Total	Mg	0	0
			1	1		
54	DQ	1	Total	Mg	0	0
			1	1		
54	D2	1	Total	Mg	0	0
			1	1		

- Molecule 55 is 5-(2-DIETHYLAMINO-ETHANESULFONYL)-21-HYDROXY-10-ISOPROPYL-11,19-DIMETHYL-9,26-DIOXA-3,15,28-TRIAZA-TRICYCLO[23.2.1.00,255]OCTACOSA-1(27),12,17,19,25(28)-PENTAENE-2,8,14,23-TETRAONE (CCD ID: DOL) (formula: C₃₄H₅₀N₄O₉S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
55	BA	1	Total	C	N	O	S	0	0
			48	34	4	9	1		
55	DA	1	Total	C	N	O	S	0	0
			48	34	4	9	1		

- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	B4	1	Total	Zn	0	0
			1	1		
56	D4	1	Total	Zn	0	0
			1	1		

- Molecule 57 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	AA	195	Total	O	0	0
			195	195		
57	AE	1	Total	O	0	0
			1	1		
57	AL	1	Total	O	0	0
			1	1		
57	AN	3	Total	O	0	0
			3	3		
57	AT	2	Total	O	0	0
			2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	AU	1	Total O 1 1	0	0
57	BA	615	Total O 615 615	0	0
57	BB	13	Total O 13 13	0	0
57	BC	8	Total O 8 8	0	0
57	BD	3	Total O 3 3	0	0
57	BE	2	Total O 2 2	0	0
57	BF	1	Total O 1 1	0	0
57	BL	7	Total O 7 7	0	0
57	BN	5	Total O 5 5	0	0
57	BQ	1	Total O 1 1	0	0
57	BS	1	Total O 1 1	0	0
57	BT	1	Total O 1 1	0	0
57	BU	1	Total O 1 1	0	0
57	BV	1	Total O 1 1	0	0
57	B2	1	Total O 1 1	0	0
57	B3	3	Total O 3 3	0	0
57	B4	2	Total O 2 2	0	0
57	CA	193	Total O 193 193	0	0
57	CL	1	Total O 1 1	0	0
57	CN	1	Total O 1 1	0	0
57	CT	2	Total O 2 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	CU	1	Total 1	O 1	0	0
57	DA	608	Total 608	O 608	0	0
57	DB	13	Total 13	O 13	0	0
57	DC	10	Total 10	O 10	0	0
57	DD	4	Total 4	O 4	0	0
57	DE	4	Total 4	O 4	0	0
57	DJ	1	Total 1	O 1	0	0
57	DL	4	Total 4	O 4	0	0
57	DN	2	Total 2	O 2	0	0
57	DS	2	Total 2	O 2	0	0
57	DT	3	Total 3	O 3	0	0
57	DU	1	Total 1	O 1	0	0
57	DV	1	Total 1	O 1	0	0
57	D2	1	Total 1	O 1	0	0
57	D3	1	Total 1	O 1	0	0
57	D4	1	Total 1	O 1	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	210.21Å 433.03Å 619.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.97 – 2.90 39.97 – 2.90	Depositor EDS
% Data completeness (in resolution range)	94.9 (39.97-2.90) 94.9 (39.97-2.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 2.90Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.220 , 0.264 0.222 , 0.265	Depositor DCC
R_{free} test set	4701 reflections (0.40%)	wwPDB-VP
Wilson B-factor (Å ²)	44.0	Xtriage
Anisotropy	0.529	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 46.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	288276	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.55% 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 501 ligands modelled in this entry, 499 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
55	DOL	DA	3001	-	47,50,50	3.31	17 (36%)	57,70,70	2.89	18 (31%)
55	DOL	BA	3001	-	47,50,50	3.17	19 (40%)	57,70,70	2.89	19 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	DOL	DA	3001	-	-	15/64/77/77	0/2/3/3
55	DOL	BA	3001	-	-	18/64/77/77	0/2/3/3

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	DA	3001	DOL	C10-N9	9.87	1.39	1.29
55	DA	3001	DOL	O15-C14	8.97	1.37	1.21
55	BA	3001	DOL	O15-C14	8.85	1.37	1.21
55	BA	3001	DOL	C10-N9	8.80	1.38	1.29
55	DA	3001	DOL	C22-C23	7.50	1.52	1.32
55	DA	3001	DOL	C6-N5	7.18	1.45	1.34
55	BA	3001	DOL	C6-N5	7.08	1.45	1.34
55	BA	3001	DOL	C22-C23	6.77	1.50	1.32
55	BA	3001	DOL	O38-C37	6.54	1.37	1.21
55	DA	3001	DOL	C26-N25	6.52	1.47	1.34
55	DA	3001	DOL	O38-C37	6.47	1.37	1.21
55	DA	3001	DOL	C19-C20	6.22	1.51	1.34
55	BA	3001	DOL	C19-C20	5.80	1.49	1.34
55	BA	3001	DOL	C26-N25	5.41	1.45	1.34
55	DA	3001	DOL	C28-C29	3.84	1.41	1.32
55	BA	3001	DOL	O36-C32	-3.60	1.39	1.44
55	BA	3001	DOL	C3-C2	-3.58	1.48	1.54
55	DA	3001	DOL	O18-C17	-3.54	1.37	1.43
55	BA	3001	DOL	C28-C29	3.54	1.40	1.32
55	DA	3001	DOL	C3-C2	-3.33	1.49	1.54
55	BA	3001	DOL	O18-C17	-3.19	1.38	1.43
55	BA	3001	DOL	C12-C8	3.18	1.38	1.34
55	DA	3001	DOL	C12-C8	3.08	1.37	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	BA	3001	DOL	O36-C37	-3.03	1.27	1.34
55	DA	3001	DOL	O36-C32	-2.91	1.40	1.44
55	BA	3001	DOL	C16-C17	-2.90	1.48	1.54
55	DA	3001	DOL	C22-C20	2.85	1.52	1.46
55	BA	3001	DOL	C3-C4	2.55	1.57	1.52
55	DA	3001	DOL	C16-C17	-2.48	1.49	1.54
55	DA	3001	DOL	O36-C37	-2.34	1.29	1.34
55	BA	3001	DOL	C1-N5	-2.20	1.43	1.46
55	DA	3001	DOL	C8-C6	2.15	1.52	1.49
55	BA	3001	DOL	C22-C20	2.13	1.50	1.46
55	BA	3001	DOL	C8-C6	2.06	1.52	1.49
55	DA	3001	DOL	C3-C4	2.03	1.56	1.52
55	BA	3001	DOL	C30-C32	-2.02	1.49	1.54

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	DA	3001	DOL	O40-S39-O41	-15.62	100.41	118.13
55	BA	3001	DOL	O40-S39-O41	-11.61	104.96	118.13
55	BA	3001	DOL	O11-C10-C13	7.91	125.01	117.70
55	BA	3001	DOL	C29-C28-C26	-7.79	104.35	122.67
55	BA	3001	DOL	C43-C42-S39	6.81	126.83	112.38
55	DA	3001	DOL	O11-C10-C13	5.50	122.79	117.70
55	DA	3001	DOL	C4-N5-C1	-5.39	106.19	112.51
55	BA	3001	DOL	C24-N25-C26	-4.62	114.69	122.17
55	DA	3001	DOL	C30-C29-C28	-4.36	114.77	126.30
55	DA	3001	DOL	C23-C22-C20	-4.13	119.65	125.89
55	DA	3001	DOL	C29-C28-C26	-3.86	113.59	122.67
55	DA	3001	DOL	C32-O36-C37	3.64	123.81	117.76
55	BA	3001	DOL	O7-C6-N5	-3.45	115.41	122.17
55	BA	3001	DOL	C4-N5-C1	-3.23	108.72	112.51
55	DA	3001	DOL	O36-C37-C1	3.21	117.96	111.48
55	BA	3001	DOL	C12-C8-N9	3.15	111.49	109.15
55	BA	3001	DOL	C28-C26-N25	3.02	121.69	115.07
55	DA	3001	DOL	O41-S39-C2	2.94	111.34	108.50
55	BA	3001	DOL	O27-C26-N25	-2.90	117.75	122.29
55	BA	3001	DOL	C2-C1-C37	-2.87	103.89	113.62
55	BA	3001	DOL	O40-S39-C42	2.75	117.31	108.00
55	BA	3001	DOL	O36-C37-C1	2.73	116.99	111.48
55	DA	3001	DOL	O11-C10-N9	-2.71	111.16	114.09
55	BA	3001	DOL	C23-C22-C20	-2.68	121.84	125.89
55	BA	3001	DOL	C12-C8-C6	-2.68	122.57	127.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	BA	3001	DOL	C30-C29-C28	-2.67	119.25	126.30
55	DA	3001	DOL	C12-C8-N9	2.61	111.09	109.15
55	BA	3001	DOL	C21-C20-C22	2.51	121.92	118.09
55	BA	3001	DOL	O11-C10-N9	-2.48	111.41	114.09
55	BA	3001	DOL	O15-C14-C13	-2.34	117.59	121.20
55	DA	3001	DOL	O40-S39-C2	2.33	110.75	108.50
55	DA	3001	DOL	C3-C4-N5	-2.27	100.73	103.22
55	DA	3001	DOL	C43-C42-S39	2.26	117.16	112.38
55	DA	3001	DOL	C12-C8-C6	-2.25	123.38	127.60
55	DA	3001	DOL	C17-C16-C14	-2.07	109.55	113.90
55	DA	3001	DOL	C31-C30-C32	2.05	114.71	111.11
55	DA	3001	DOL	O38-C37-C1	-2.01	120.74	124.58

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	BA	3001	DOL	C43-C42-S39-O41
55	BA	3001	DOL	C43-C42-S39-O40
55	BA	3001	DOL	S39-C42-C43-N44
55	BA	3001	DOL	O11-C10-C13-C14
55	DA	3001	DOL	C3-C2-S39-O40
55	DA	3001	DOL	O11-C10-C13-C14
55	BA	3001	DOL	N25-C26-C28-C29
55	BA	3001	DOL	O27-C26-C28-C29
55	DA	3001	DOL	N25-C26-C28-C29
55	BA	3001	DOL	C21-C20-C22-C23
55	BA	3001	DOL	C19-C20-C22-C23
55	DA	3001	DOL	C28-C29-C30-C31
55	DA	3001	DOL	O27-C26-C28-C29
55	DA	3001	DOL	C46-C45-N44-C47
55	BA	3001	DOL	C46-C45-N44-C43
55	BA	3001	DOL	C46-C45-N44-C47
55	DA	3001	DOL	C46-C45-N44-C43
55	DA	3001	DOL	N9-C10-C13-C14
55	DA	3001	DOL	C2-C1-C37-O38
55	DA	3001	DOL	C2-C1-C37-O36
55	DA	3001	DOL	C10-C13-C14-O15
55	BA	3001	DOL	C43-C42-S39-C2
55	DA	3001	DOL	C43-C42-S39-C2
55	DA	3001	DOL	C10-C13-C14-C16
55	BA	3001	DOL	O36-C32-C33-C34

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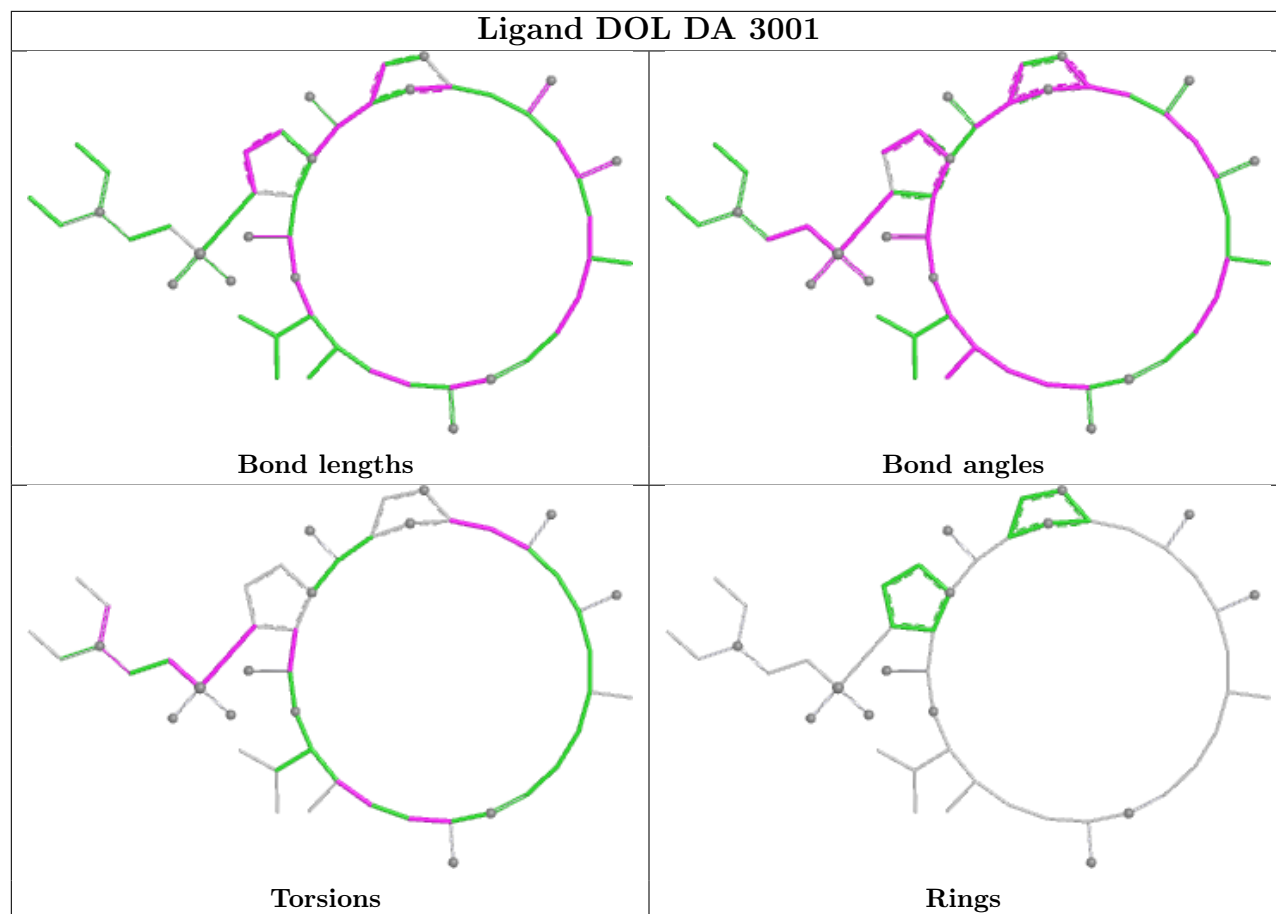
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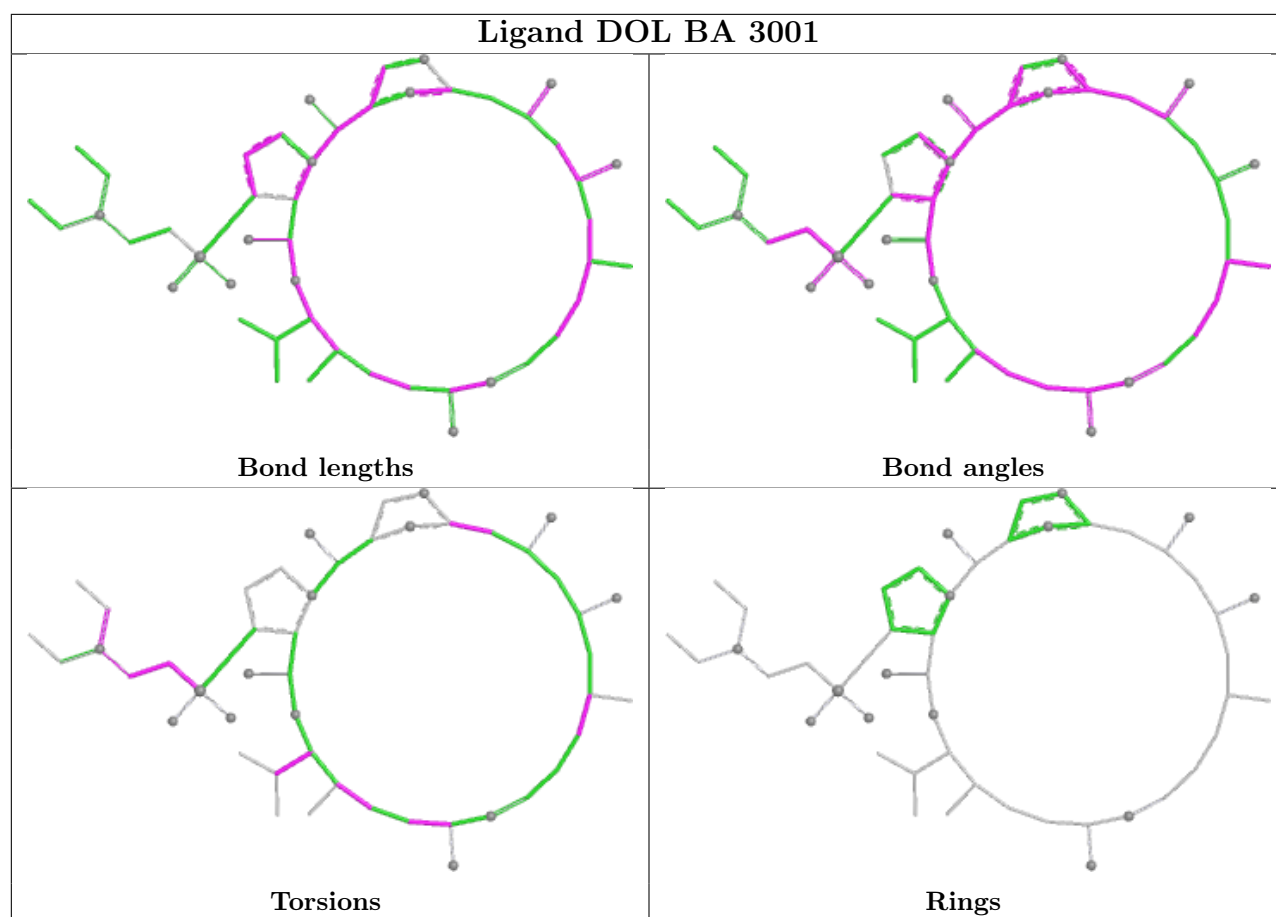
Mol	Chain	Res	Type	Atoms
55	BA	3001	DOL	N9-C10-C13-C14
55	BA	3001	DOL	C28-C29-C30-C31
55	BA	3001	DOL	C42-C43-N44-C45
55	DA	3001	DOL	C42-C43-N44-C47
55	BA	3001	DOL	C30-C32-C33-C35
55	BA	3001	DOL	O36-C32-C33-C35
55	BA	3001	DOL	C42-C43-N44-C47
55	DA	3001	DOL	C1-C2-S39-C42

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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	1538/1539 (99%)	-0.11	25 (1%) 70 62	11, 51, 132, 183	0
1	CA	1539/1539 (100%)	0.38	81 (5%) 32 25	24, 70, 147, 178	0
2	AB	218/218 (100%)	1.05	29 (13%) 7 6	40, 75, 101, 117	0
2	CB	218/218 (100%)	1.12	30 (13%) 6 5	60, 88, 108, 123	0
3	AC	206/206 (100%)	0.33	8 (3%) 43 35	37, 58, 80, 95	0
3	CC	206/206 (100%)	0.94	23 (11%) 10 9	55, 80, 98, 108	0
4	AD	205/205 (100%)	0.57	14 (6%) 23 18	33, 57, 80, 100	0
4	CD	205/205 (100%)	0.06	8 (3%) 43 35	15, 36, 60, 84	0
5	AE	150/150 (100%)	0.37	9 (6%) 27 21	29, 48, 78, 94	0
5	CE	150/150 (100%)	0.64	8 (5%) 32 25	27, 53, 83, 104	0
6	AF	100/100 (100%)	0.51	3 (3%) 52 43	35, 56, 75, 79	0
6	CF	100/100 (100%)	0.62	4 (4%) 42 34	43, 73, 92, 104	0
7	AG	151/151 (100%)	0.84	13 (8%) 16 13	54, 76, 92, 100	0
7	CG	151/151 (100%)	1.92	66 (43%) 0 0	82, 106, 115, 119	0
8	AH	129/129 (100%)	0.19	2 (1%) 70 62	29, 48, 68, 79	0
8	CH	129/129 (100%)	0.49	4 (3%) 51 42	48, 64, 81, 96	0
9	AI	127/127 (100%)	1.12	18 (14%) 6 5	45, 75, 98, 107	0
9	CI	127/127 (100%)	1.71	45 (35%) 1 1	81, 97, 114, 121	0
10	AJ	98/98 (100%)	1.07	13 (13%) 7 6	41, 68, 88, 116	0
10	CJ	98/98 (100%)	1.95	42 (42%) 0 0	73, 98, 115, 124	0
11	AK	117/117 (100%)	0.80	9 (7%) 19 16	28, 62, 92, 120	0
11	CK	117/117 (100%)	0.50	1 (0%) 81 75	36, 68, 82, 90	0
12	AL	123/123 (100%)	0.17	8 (6%) 25 20	20, 35, 65, 97	0
12	CL	123/123 (100%)	0.67	10 (8%) 18 15	33, 50, 75, 96	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
13	AM	114/114 (100%)	1.06	14 (12%)	8	7	49, 72, 93, 104	0
13	CM	114/114 (100%)	2.18	58 (50%)	0	0	94, 115, 124, 126	0
14	AN	96/100 (96%)	1.10	13 (13%)	7	5	41, 62, 96, 105	0
14	CN	96/100 (96%)	2.01	41 (42%)	0	0	71, 97, 116, 123	0
15	AO	88/88 (100%)	0.45	3 (3%)	48	39	31, 48, 65, 90	0
15	CO	88/88 (100%)	0.56	3 (3%)	48	39	37, 65, 80, 103	0
16	AP	82/82 (100%)	0.48	4 (4%)	35	27	35, 48, 84, 109	0
16	CP	82/82 (100%)	0.96	9 (10%)	10	9	45, 62, 92, 113	0
17	AQ	80/80 (100%)	0.51	4 (5%)	34	27	28, 49, 75, 110	0
17	CQ	80/80 (100%)	0.98	8 (10%)	12	10	43, 79, 98, 100	0
18	AR	55/55 (100%)	0.79	7 (12%)	8	6	42, 55, 78, 101	0
18	CR	55/55 (100%)	0.46	3 (5%)	30	24	36, 55, 78, 109	0
19	AS	79/79 (100%)	1.14	12 (15%)	5	4	56, 72, 89, 97	0
19	CS	79/79 (100%)	2.36	45 (56%)	0	0	98, 115, 124, 129	0
20	AT	85/85 (100%)	0.65	8 (9%)	14	12	36, 48, 70, 95	0
20	CT	85/85 (100%)	1.69	21 (24%)	2	1	54, 78, 96, 101	0
21	AU	51/51 (100%)	1.49	12 (23%)	2	2	44, 76, 97, 105	0
21	CU	51/51 (100%)	1.45	13 (25%)	1	1	45, 71, 100, 103	0
22	BA	2897/2903 (99%)	-0.64	142 (4%)	35	27	1, 14, 129, 195	0
22	DA	2897/2903 (99%)	0.78	175 (6%)	27	21	41, 85, 148, 181	0
23	BB	119/119 (100%)	-0.81	0	100	100	2, 23, 50, 80	0
23	DB	118/119 (99%)	0.87	5 (4%)	40	32	69, 115, 134, 143	0
24	BC	271/271 (100%)	-0.32	5 (1%)	67	59	2, 20, 37, 55	0
24	DC	271/271 (100%)	0.92	29 (10%)	11	9	47, 64, 77, 96	0
25	BD	209/209 (100%)	-0.60	1 (0%)	87	83	0, 10, 36, 65	0
25	DD	209/209 (100%)	1.06	27 (12%)	7	6	53, 72, 88, 96	0
26	BE	201/201 (100%)	-0.41	0	100	100	2, 24, 55, 88	0
26	DE	201/201 (100%)	1.49	48 (23%)	2	2	53, 90, 107, 114	0
27	BF	177/177 (100%)	0.24	5 (2%)	55	46	22, 44, 76, 90	0
27	DF	177/177 (100%)	2.01	76 (42%)	0	0	97, 114, 126, 131	0
28	BG	176/176 (100%)	-0.26	0	100	100	16, 36, 57, 72	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DG	176/176 (100%)	1.51	36 (20%) 2 2	77, 96, 111, 121	0
29	BH	149/149 (100%)	2.31	78 (52%) 0 0	25, 102, 121, 129	0
29	DH	149/149 (100%)	1.58	50 (33%) 1 1	25, 92, 107, 115	0
30	BI	141/141 (100%)	2.41	80 (56%) 0 0	90, 117, 127, 134	0
30	DI	141/141 (100%)	2.92	92 (65%) 0 0	105, 126, 137, 143	0
31	BJ	142/142 (100%)	-0.62	0 100 100	1, 6, 23, 36	0
31	DJ	142/142 (100%)	0.91	19 (13%) 7 5	52, 69, 83, 91	0
32	BK	122/122 (100%)	-0.50	2 (1%) 70 62	3, 12, 31, 62	0
32	DK	122/122 (100%)	0.84	12 (9%) 13 11	48, 66, 84, 96	0
33	BL	143/143 (100%)	-0.30	2 (1%) 73 65	1, 19, 43, 65	0
33	DL	143/143 (100%)	1.92	53 (37%) 1 0	46, 87, 99, 115	0
34	BM	136/136 (100%)	-0.59	0 100 100	1, 10, 30, 83	0
34	DM	136/136 (100%)	0.83	10 (7%) 20 17	42, 71, 86, 100	0
35	BN	120/120 (100%)	-0.62	0 100 100	3, 8, 18, 63	0
35	DN	120/120 (100%)	1.58	36 (30%) 1 1	59, 79, 94, 112	0
36	BO	116/116 (100%)	-0.31	0 100 100	14, 26, 45, 55	0
36	DO	116/116 (100%)	1.68	45 (38%) 1 0	86, 100, 111, 118	0
37	BP	114/114 (100%)	-0.43	1 (0%) 81 75	8, 17, 41, 72	0
37	DP	114/114 (100%)	0.97	11 (9%) 13 11	61, 75, 86, 95	0
38	BQ	117/117 (100%)	-0.58	0 100 100	0, 3, 13, 34	0
38	DQ	117/117 (100%)	1.47	28 (23%) 2 2	57, 71, 80, 89	0
39	BR	103/103 (100%)	-0.41	0 100 100	1, 13, 30, 58	0
39	DR	103/103 (100%)	1.35	20 (19%) 3 2	58, 81, 94, 104	0
40	BS	110/110 (100%)	-0.56	0 100 100	2, 5, 24, 66	0
40	DS	110/110 (100%)	1.37	25 (22%) 2 2	62, 80, 95, 106	0
41	BT	93/93 (100%)	0.00	5 (5%) 31 24	9, 26, 68, 100	0
41	DT	93/93 (100%)	1.94	40 (43%) 0 0	73, 92, 106, 115	0
42	BU	102/102 (100%)	-0.10	4 (3%) 43 35	12, 29, 63, 79	0
42	DU	102/102 (100%)	2.23	52 (50%) 0 0	78, 96, 110, 122	0
43	BV	94/94 (100%)	-0.43	0 100 100	5, 21, 43, 55	0
43	DV	94/94 (100%)	1.02	9 (9%) 13 11	74, 88, 99, 106	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BW	76/76 (100%)	-0.48	1 (1%) 75 67	5, 12, 30, 57	0
44	DW	75/76 (98%)	1.30	15 (20%) 3 2	58, 83, 92, 105	0
45	BX	77/77 (100%)	-0.30	0 100 100	8, 22, 51, 68	0
45	DX	77/77 (100%)	1.28	14 (18%) 3 3	50, 72, 87, 92	0
46	BY	63/63 (100%)	0.34	3 (4%) 35 28	24, 41, 73, 95	0
46	DY	63/63 (100%)	1.94	29 (46%) 0 0	82, 99, 107, 110	0
47	BZ	58/58 (100%)	-0.49	0 100 100	2, 9, 29, 35	0
47	DZ	58/58 (100%)	1.12	10 (17%) 4 3	60, 74, 85, 103	0
48	B0	56/56 (100%)	-0.58	0 100 100	1, 10, 35, 60	0
48	D0	56/56 (100%)	1.55	15 (26%) 1 1	52, 83, 98, 105	0
49	B1	50/50 (100%)	-0.28	0 100 100	15, 27, 51, 58	0
49	D1	50/50 (100%)	1.75	16 (32%) 1 1	74, 90, 95, 105	0
50	B2	46/46 (100%)	-0.34	1 (2%) 62 53	5, 9, 16, 79	0
50	D2	46/46 (100%)	2.21	22 (47%) 0 0	58, 72, 87, 102	0
51	B3	64/64 (100%)	-0.58	0 100 100	4, 10, 20, 29	0
51	D3	64/64 (100%)	2.12	30 (46%) 0 0	62, 75, 84, 95	0
52	B4	38/38 (100%)	-0.26	0 100 100	8, 19, 34, 54	0
52	D4	38/38 (100%)	2.13	18 (47%) 0 0	64, 79, 90, 100	0
53	B5	191/228 (83%)	2.44	122 (63%) 0 0	100, 122, 133, 142	0
All	All	20734/20794 (99%)	0.49	2270 (10%) 10 9	0, 64, 125, 195	0

All (2270) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	CT	4	ILE	8.8
30	BI	79	LEU	8.0
30	DI	78	VAL	8.0
10	AJ	102	LEU	7.9
30	DI	54	PRO	7.9
30	BI	54	PRO	7.6
50	B2	46	LYS	7.5
29	BH	130	VAL	7.4
30	BI	53	LEU	7.4
50	D2	46	LYS	7.3
22	BA	2103	C	7.1

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Mol	Chain	Res	Type	RSRZ
30	DI	11	LEU	6.8
4	CD	25	VAL	6.7
30	BI	12	GLN	6.4
29	BH	67	ALA	6.3
30	DI	53	LEU	6.3
29	DH	142	VAL	6.2
30	DI	76	ALA	6.1
30	BI	13	VAL	6.0
22	BA	2100	G	6.0
17	AQ	20	SER	6.0
53	B5	166	ASN	5.9
7	CG	62	PHE	5.9
41	DT	34	VAL	5.9
1	CA	1536	C	5.9
22	BA	2175	C	5.9
53	B5	218	THR	5.9
22	BA	2176	A	5.9
21	AU	38	TYR	5.9
53	B5	120	VAL	5.8
12	CL	25	GLU	5.8
22	BA	2101	A	5.8
30	DI	56	PRO	5.8
22	DA	2585	U	5.8
20	AT	4	ILE	5.7
30	DI	79	LEU	5.7
29	BH	63	ALA	5.7
27	DF	32	GLU	5.7
22	BA	2132	U	5.6
7	CG	6	VAL	5.6
29	BH	94	ILE	5.6
9	CI	20	PHE	5.5
30	DI	38	PHE	5.5
38	DQ	9	ILE	5.5
19	CS	76	PRO	5.5
29	BH	121	VAL	5.4
1	CA	1538	C	5.4
29	BH	102	ALA	5.4
8	AH	2	SER	5.4
30	DI	80	LEU	5.4
13	CM	103	LYS	5.3
22	DA	2172	U	5.3
10	CJ	74	VAL	5.3

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Mol	Chain	Res	Type	RSRZ
22	BA	1072	C	5.3
30	BI	56	PRO	5.3
29	BH	131	SER	5.2
41	DT	41	ALA	5.2
30	BI	11	LEU	5.2
30	DI	68	THR	5.2
22	BA	2102	G	5.2
33	DL	27	LEU	5.2
38	DQ	8	VAL	5.2
29	BH	81	ALA	5.2
30	DI	133	ALA	5.2
30	DI	118	THR	5.1
22	BA	2184	A	5.1
33	DL	19	LEU	5.1
24	DC	242	LYS	5.1
30	BI	15	ALA	5.1
53	B5	140	ASN	5.1
30	DI	27	ALA	5.1
36	DO	32	PRO	5.1
51	D3	57	LEU	5.0
22	BA	2123	G	5.0
30	BI	2	ALA	5.0
53	B5	165	ARG	5.0
2	CB	135	LEU	5.0
3	CC	37	PHE	5.0
42	DU	71	ALA	5.0
29	BH	97	ARG	5.0
13	CM	7	ILE	4.9
30	DI	14	ALA	4.9
51	D3	15	LYS	4.9
42	DU	52	LEU	4.9
50	D2	42	LEU	4.9
30	DI	55	ILE	4.9
29	BH	98	ASP	4.9
19	CS	37	ARG	4.9
53	B5	216	THR	4.9
53	B5	76	LEU	4.9
14	CN	2	ALA	4.9
30	DI	83	ALA	4.9
7	AG	5	ARG	4.9
21	CU	35	ARG	4.9
10	CJ	102	LEU	4.8

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Mol	Chain	Res	Type	RSRZ
27	DF	67	ILE	4.8
30	BI	86	ILE	4.8
42	DU	67	VAL	4.8
22	BA	2178	C	4.8
24	DC	238	ARG	4.8
51	D3	61	CYS	4.8
2	AB	157	LEU	4.8
49	D1	24	THR	4.8
30	DI	13	VAL	4.8
20	AT	68	HIS	4.8
22	BA	2172	U	4.8
12	CL	124	ALA	4.8
21	CU	38	TYR	4.8
30	DI	23	PRO	4.8
41	DT	36	LYS	4.7
41	DT	57	VAL	4.7
29	BH	119	ASN	4.7
34	DM	99	GLY	4.7
24	DC	205	LEU	4.7
13	CM	45	ILE	4.7
22	BA	2148	G	4.7
2	CB	32	PHE	4.7
14	CN	8	ALA	4.7
26	DE	119	ILE	4.7
50	D2	33	ARG	4.7
53	B5	217	THR	4.7
45	DX	49	LEU	4.7
22	BA	1094	U	4.7
22	BA	2185	U	4.7
30	DI	129	ILE	4.7
20	CT	68	HIS	4.7
33	DL	49	GLY	4.7
1	CA	1539	C	4.7
19	CS	49	ILE	4.6
30	BI	78	VAL	4.6
22	BA	2585	U	4.6
30	DI	24	VAL	4.6
33	DL	70	LYS	4.6
19	CS	74	PHE	4.6
22	BA	2136	G	4.6
22	DA	1606	C	4.6
3	AC	175	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
2	AB	156	GLY	4.6
4	AD	37	ALA	4.6
30	DI	4	LYS	4.6
14	CN	48	LEU	4.6
17	AQ	5	ILE	4.6
20	CT	8	LYS	4.6
25	DD	126	ASN	4.6
30	BI	27	ALA	4.5
48	D0	2	ALA	4.5
53	B5	205	ALA	4.5
22	BA	2177	C	4.5
22	DA	931	U	4.5
27	DF	79	ILE	4.5
53	B5	142	LYS	4.5
14	CN	51	LEU	4.5
35	DN	46	ARG	4.5
53	B5	211	ARG	4.5
30	BI	88	SER	4.5
30	BI	55	ILE	4.4
36	DO	4	LYS	4.4
12	CL	38	TYR	4.4
22	BA	2174	C	4.4
53	B5	179	ALA	4.4
27	DF	76	GLY	4.4
39	DR	75	VAL	4.4
25	DD	128	ARG	4.4
13	CM	31	LYS	4.4
13	CM	86	TYR	4.4
30	DI	5	VAL	4.4
33	DL	14	LYS	4.4
38	DQ	22	LYS	4.4
4	CD	24	GLY	4.4
1	CA	1535	C	4.4
13	CM	63	PHE	4.4
42	DU	3	ALA	4.4
42	DU	80	ALA	4.3
27	DF	35	THR	4.3
20	CT	9	LYS	4.3
10	CJ	100	ILE	4.3
26	DE	73	ILE	4.3
13	CM	18	ALA	4.3
53	B5	97	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
48	D0	27	SER	4.3
10	CJ	43	PRO	4.3
27	DF	25	VAL	4.3
30	DI	2	ALA	4.3
22	BA	2130	U	4.3
29	DH	108	VAL	4.3
30	BI	133	ALA	4.3
7	CG	5	ARG	4.3
33	DL	68	SER	4.3
38	DQ	2	ALA	4.3
22	BA	1093	G	4.2
22	BA	2152	G	4.2
22	DA	2174	C	4.2
29	BH	115	VAL	4.2
53	B5	141	PRO	4.2
46	DY	56	LEU	4.2
29	BH	120	GLY	4.2
41	DT	43	ILE	4.2
22	BA	2121	G	4.2
29	BH	62	LEU	4.2
24	BC	237	GLY	4.2
29	BH	72	ILE	4.2
30	DI	109	ILE	4.2
53	B5	50	ILE	4.2
1	CA	1537	U	4.2
7	CG	32	VAL	4.2
30	BI	22	PRO	4.2
29	BH	111	ALA	4.2
1	AA	1535	C	4.2
11	CK	126	LYS	4.2
52	D4	12	ARG	4.2
22	BA	1926	U	4.2
22	BA	2182	U	4.2
29	BH	117	LEU	4.2
29	BH	146	VAL	4.2
30	DI	28	LEU	4.2
36	DO	57	ALA	4.2
29	BH	101	ASP	4.2
50	D2	22	MET	4.2
9	AI	129	LYS	4.1
22	BA	2124	G	4.1
22	BA	2141	G	4.1

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Mol	Chain	Res	Type	RSRZ
29	BH	122	LEU	4.1
30	BI	80	LEU	4.1
30	DI	9	VAL	4.1
22	DA	12	U	4.1
46	DY	24	GLU	4.1
25	DD	154	LYS	4.1
30	DI	82	LYS	4.1
7	CG	7	ILE	4.1
33	DL	73	ILE	4.1
53	B5	145	THR	4.1
50	D2	23	ALA	4.1
27	DF	44	ILE	4.1
27	DF	136	ILE	4.1
21	CU	14	VAL	4.1
42	BU	55	PRO	4.1
30	BI	91	GLY	4.1
52	D4	26	ILE	4.1
1	CA	1302	C	4.1
14	CN	58	SER	4.1
22	DA	1093	G	4.1
33	DL	79	LEU	4.0
30	DI	70	VAL	4.0
30	DI	7	ALA	4.0
3	CC	162	ILE	4.0
37	BP	2	SER	4.0
30	DI	58	VAL	4.0
22	BA	2186	G	4.0
30	BI	81	LYS	4.0
46	DY	19	LEU	4.0
1	CA	1320	C	4.0
14	CN	34	VAL	4.0
4	AD	151	LYS	4.0
4	CD	27	ALA	4.0
35	DN	97	ILE	4.0
53	B5	84	ILE	4.0
52	D4	21	GLY	4.0
22	BA	1087	G	4.0
22	BA	2885	G	4.0
27	DF	88	LYS	4.0
30	DI	22	PRO	4.0
10	CJ	75	ASP	4.0
27	DF	54	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
29	DH	84	ALA	4.0
9	CI	68	LYS	4.0
22	BA	2193	G	4.0
30	DI	81	LYS	4.0
20	CT	7	ALA	3.9
29	BH	69	ALA	3.9
36	DO	8	ILE	3.9
42	DU	39	ILE	3.9
50	D2	18	PHE	3.9
49	D1	38	LYS	3.9
49	D1	53	LYS	3.9
22	DA	1073	A	3.9
29	BH	110	VAL	3.9
51	D3	26	HIS	3.9
42	DU	50	PRO	3.9
9	AI	43	THR	3.9
30	BI	115	ALA	3.9
30	DI	130	GLU	3.9
10	CJ	71	LEU	3.9
42	DU	14	LEU	3.9
53	B5	65	LEU	3.9
41	DT	9	LYS	3.9
7	AG	6	VAL	3.9
13	CM	10	PRO	3.9
45	DX	35	SER	3.9
30	DI	59	ILE	3.9
30	DI	106	LEU	3.9
33	DL	92	LEU	3.9
49	D1	36	LEU	3.9
2	AB	136	MET	3.9
10	CJ	77	VAL	3.9
22	BA	2160	C	3.9
53	B5	23	ILE	3.9
30	DI	114	ALA	3.9
53	B5	199	ALA	3.9
33	DL	11	GLY	3.9
33	DL	84	LYS	3.9
36	DO	68	LYS	3.9
53	B5	193	PHE	3.9
9	CI	119	ARG	3.9
20	CT	24	ARG	3.9
29	BH	68	ARG	3.9

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Mol	Chain	Res	Type	RSRZ
30	DI	35	ILE	3.9
45	DX	50	ARG	3.9
30	BI	14	ALA	3.9
35	DN	25	ALA	3.9
20	CT	69	LYS	3.8
1	CA	1362	A	3.8
1	CA	1235	U	3.8
40	DS	86	MET	3.8
30	BI	5	VAL	3.8
30	DI	86	ILE	3.8
50	D2	35	ARG	3.8
38	DQ	7	GLY	3.8
41	BT	93	LEU	3.8
7	CG	43	VAL	3.8
22	BA	2098	U	3.8
13	CM	101	ARG	3.8
14	AN	30	ILE	3.8
29	BH	99	ILE	3.8
9	CI	64	TYR	3.8
19	CS	71	LEU	3.8
33	DL	26	GLY	3.8
36	DO	65	THR	3.8
19	CS	51	VAL	3.8
53	B5	63	VAL	3.8
53	B5	66	PRO	3.8
3	CC	193	TYR	3.8
53	B5	192	ALA	3.8
46	DY	18	LEU	3.8
46	DY	22	LEU	3.8
38	DQ	29	SER	3.8
1	AA	1538	C	3.8
1	CA	1305	G	3.8
22	BA	2147	A	3.8
22	BA	2183	A	3.8
33	DL	61	LEU	3.8
40	DS	46	LEU	3.8
42	DU	15	THR	3.8
39	DR	37	GLU	3.7
38	DQ	11	ARG	3.7
27	DF	156	ILE	3.7
42	DU	12	ILE	3.7
26	DE	36	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
28	DG	150	ALA	3.7
30	BI	114	ALA	3.7
33	DL	71	ALA	3.7
22	BA	2180	U	3.7
27	DF	66	LEU	3.7
27	DF	82	GLY	3.7
9	CI	128	SER	3.7
27	DF	28	VAL	3.7
28	DG	168	VAL	3.7
32	DK	35	VAL	3.7
40	DS	45	VAL	3.7
53	B5	73	VAL	3.7
19	CS	30	PRO	3.7
14	AN	44	ALA	3.7
19	CS	31	LEU	3.7
33	DL	72	ALA	3.7
14	CN	20	TYR	3.7
22	BA	2192	U	3.7
30	DI	42	PHE	3.7
36	DO	66	GLY	3.7
22	DA	1072	C	3.7
22	BA	1171	G	3.7
11	AK	126	LYS	3.7
42	DU	5	ILE	3.7
33	DL	62	PRO	3.7
4	AD	27	ALA	3.7
7	CG	66	LEU	3.7
30	DI	138	LEU	3.7
20	CT	3	ASN	3.7
30	BI	8	TYR	3.7
53	B5	111	PHE	3.7
22	BA	1923	U	3.7
22	BA	2145	C	3.7
24	DC	228	VAL	3.7
53	B5	172	ILE	3.7
30	DI	77	ALA	3.7
4	AD	28	ILE	3.7
7	CG	38	THR	3.7
10	CJ	44	THR	3.7
27	DF	31	VAL	3.7
30	BI	118	THR	3.7
1	AA	1536	C	3.6

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Mol	Chain	Res	Type	RSRZ
19	CS	15	LEU	3.6
22	BA	885	C	3.6
22	BA	2104	C	3.6
33	DL	80	SER	3.6
38	DQ	59	GLN	3.6
22	BA	2112	G	3.6
14	CN	69	ARG	3.6
39	DR	88	GLY	3.6
53	B5	96	GLY	3.6
7	CG	27	VAL	3.6
30	BI	140	VAL	3.6
33	DL	101	ILE	3.6
13	CM	55	THR	3.6
22	BA	2155	U	3.6
21	CU	16	LEU	3.6
7	CG	134	ALA	3.6
22	BA	1069	A	3.6
29	BH	85	GLY	3.6
7	CG	75	VAL	3.6
49	D1	42	VAL	3.6
29	BH	96	THR	3.6
53	B5	41	THR	3.6
10	CJ	41	PRO	3.6
31	DJ	47	HIS	3.6
13	CM	27	LYS	3.6
30	BI	4	LYS	3.6
40	DS	83	LYS	3.6
6	CF	80	PHE	3.6
44	DW	52	GLY	3.6
22	DA	331	C	3.6
13	CM	16	VAL	3.6
17	AQ	83	VAL	3.6
36	DO	103	VAL	3.6
42	DU	13	VAL	3.6
18	AR	51	TYR	3.6
30	DI	60	THR	3.6
33	DL	74	THR	3.6
19	AS	5	LEU	3.6
51	D3	49	MET	3.6
1	AA	121	U	3.6
22	BA	2125	G	3.6
12	AL	124	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
26	DE	88	ARG	3.6
40	DS	84	ARG	3.6
17	CQ	20	SER	3.6
42	DU	20	GLY	3.6
52	D4	23	ILE	3.6
7	CG	105	VAL	3.6
22	BA	2179	C	3.6
22	DA	2175	C	3.6
41	DT	60	THR	3.6
46	DY	43	LEU	3.6
53	B5	121	MET	3.6
24	DC	39	LYS	3.5
30	BI	82	LYS	3.5
33	DL	29	LYS	3.5
39	DR	76	LYS	3.5
9	AI	17	ALA	3.5
26	DE	49	ARG	3.5
30	BI	83	ALA	3.5
33	DL	78	ARG	3.5
22	BA	2156	G	3.5
24	DC	49	ILE	3.5
26	DE	96	VAL	3.5
29	BH	149	GLU	3.5
10	AJ	75	ASP	3.5
40	DS	94	ASP	3.5
53	B5	137	LEU	3.5
30	DI	10	LYS	3.5
14	CN	61	ARG	3.5
14	CN	60	GLN	3.5
30	DI	110	ALA	3.5
14	CN	30	ILE	3.5
49	D1	48	ILE	3.5
53	B5	147	GLY	3.5
28	DG	62	TRP	3.5
29	BH	83	LYS	3.5
14	CN	70	PRO	3.5
30	BI	26	PRO	3.5
30	DI	74	PRO	3.5
10	CJ	94	ALA	3.5
41	DT	46	ALA	3.5
30	DI	12	GLN	3.5
30	DI	49	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
22	BA	2149	U	3.5
53	B5	44	VAL	3.5
44	DW	44	LYS	3.5
14	CN	53	ARG	3.5
20	AT	36	TYR	3.5
22	BA	2107	G	3.5
22	DA	75	G	3.5
7	CG	42	ILE	3.5
53	B5	78	ILE	3.5
11	AK	129	VAL	3.5
22	BA	1925	C	3.5
24	DC	235	GLY	3.5
53	B5	176	VAL	3.5
1	AA	1017	U	3.5
22	BA	2099	U	3.5
27	DF	72	LYS	3.5
52	D4	15	LYS	3.5
52	D4	18	LYS	3.5
53	B5	178	LYS	3.5
29	BH	118	PRO	3.5
30	BI	23	PRO	3.5
46	DY	48	ARG	3.5
28	DG	174	ALA	3.5
53	B5	77	ALA	3.5
1	CA	1242	G	3.4
22	BA	2159	G	3.4
7	CG	112	GLY	3.4
2	CB	132	LYS	3.4
9	CI	111	VAL	3.4
30	BI	24	VAL	3.4
33	DL	28	GLY	3.4
7	CG	23	LEU	3.4
13	CM	89	LEU	3.4
52	D4	2	LYS	3.4
2	CB	130	THR	3.4
29	BH	148	ALA	3.4
19	AS	56	GLN	3.4
10	CJ	76	ILE	3.4
13	CM	73	ILE	3.4
31	DJ	81	ILE	3.4
53	B5	38	PHE	3.4
30	BI	10	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
38	DQ	78	LYS	3.4
9	AI	54	LEU	3.4
29	DH	144	VAL	3.4
35	DN	28	LEU	3.4
24	BC	236	GLU	3.4
53	B5	155	ARG	3.4
19	CS	59	PRO	3.4
22	BA	1098	A	3.4
40	DS	80	PRO	3.4
1	CA	984	C	3.4
9	CI	108	ALA	3.4
27	DF	157	THR	3.4
12	AL	15	LYS	3.4
38	DQ	15	LYS	3.4
19	CS	60	VAL	3.4
25	DD	135	GLY	3.4
7	AG	109	ARG	3.4
40	DS	92	ARG	3.4
22	BA	2139	U	3.4
16	AP	22	ALA	3.4
22	DA	1090	A	3.4
36	DO	24	THR	3.4
6	CF	93	LYS	3.4
9	CI	7	TYR	3.4
12	AL	44	LYS	3.4
14	CN	47	LYS	3.4
20	CT	5	LYS	3.4
41	DT	82	LYS	3.4
30	DI	69	PHE	3.4
30	BI	70	VAL	3.4
51	D3	44	LEU	3.4
20	CT	63	ALA	3.4
20	CT	71	LYS	3.4
27	DF	34	ILE	3.4
51	D3	36	LYS	3.4
5	AE	31	PHE	3.4
22	DA	2126	A	3.4
22	BA	1063	G	3.3
48	D0	3	VAL	3.3
3	CC	80	LYS	3.3
14	AN	36	ALA	3.3
16	AP	81	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
26	DE	132	LYS	3.3
14	AN	21	PHE	3.3
29	BH	132	PHE	3.3
7	CG	109	ARG	3.3
30	DI	25	GLY	3.3
22	BA	2169	A	3.3
22	BA	2164	C	3.3
14	CN	57	PRO	3.3
19	CS	9	PRO	3.3
53	B5	52	PRO	3.3
13	CM	13	LYS	3.3
46	DY	44	LYS	3.3
51	D3	39	LYS	3.3
19	CS	11	ILE	3.3
29	DH	148	ALA	3.3
30	BI	76	ALA	3.3
42	DU	76	ALA	3.3
2	AB	14	VAL	3.3
24	DC	245	VAL	3.3
30	DI	128	SER	3.3
33	DL	69	ARG	3.3
38	DQ	13	ARG	3.3
53	B5	223	VAL	3.3
29	BH	70	GLU	3.3
22	DA	2309	A	3.3
1	CA	1325	C	3.3
22	DA	2124	G	3.3
10	CJ	92	LEU	3.3
38	DQ	37	GLN	3.3
3	CC	39	VAL	3.3
13	CM	60	VAL	3.3
21	AU	28	VAL	3.3
30	DI	98	VAL	3.3
30	DI	140	VAL	3.3
24	DC	213	TRP	3.3
9	CI	10	GLY	3.3
12	AL	38	TYR	3.3
27	DF	128	TYR	3.3
20	CT	33	LYS	3.3
41	DT	74	ILE	3.3
53	B5	36	ALA	3.3
28	DG	33	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
19	CS	33	THR	3.3
28	DG	36	THR	3.3
33	DL	58	TYR	3.2
53	B5	214	TYR	3.2
22	BA	1066	U	3.2
27	DF	23	ASN	3.2
30	DI	101	ILE	3.2
27	DF	70	ALA	3.2
28	DG	63	ALA	3.2
41	DT	11	LEU	3.2
30	BI	69	PHE	3.2
33	DL	107	PHE	3.2
29	BH	142	VAL	3.2
35	DN	76	VAL	3.2
52	D4	3	VAL	3.2
7	CG	133	THR	3.2
14	CN	50	THR	3.2
19	CS	34	TRP	3.2
14	CN	10	GLU	3.2
22	DA	1238	G	3.2
13	CM	22	ILE	3.2
13	CM	2	ALA	3.2
41	DT	8	LEU	3.2
53	B5	79	ALA	3.2
28	DG	153	ARG	3.2
42	DU	87	PHE	3.2
7	CG	73	VAL	3.2
7	CG	80	VAL	3.2
21	CU	53	VAL	3.2
29	BH	103	VAL	3.2
22	DA	2171	A	3.2
42	DU	19	LYS	3.2
30	BI	73	THR	3.2
22	BA	2150	C	3.2
29	BH	93	SER	3.2
29	DH	136	SER	3.2
53	B5	189	ASN	3.2
13	CM	83	LEU	3.2
26	DE	182	ALA	3.2
30	DI	134	ARG	3.2
9	AI	20	PHE	3.2
22	DA	1537	G	3.2

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Mol	Chain	Res	Type	RSRZ
30	DI	67	PHE	3.2
44	DW	60	PHE	3.2
6	AF	92	THR	3.2
28	DG	80	THR	3.2
1	CA	983	A	3.2
2	CB	136	MET	3.2
22	BA	2135	A	3.2
29	DH	149	GLU	3.2
52	D4	1	MET	3.2
18	AR	21	ILE	3.2
27	DF	106	ILE	3.2
27	DF	143	TYR	3.2
42	DU	58	ILE	3.2
19	CS	12	ASP	3.2
2	AB	129	LEU	3.2
2	CB	129	LEU	3.2
19	CS	16	LEU	3.2
22	BA	2161	C	3.2
27	DF	117	LEU	3.2
35	DN	98	LEU	3.2
44	DW	55	ARG	3.2
53	B5	69	LEU	3.2
53	B5	210	LEU	3.2
53	B5	26	ALA	3.2
4	AD	25	VAL	3.2
13	CM	43	VAL	3.2
27	DF	149	VAL	3.2
30	DI	57	VAL	3.2
33	DL	116	VAL	3.2
42	DU	44	LYS	3.2
53	B5	42	VAL	3.2
53	B5	213	VAL	3.2
22	BA	2120	G	3.2
44	DW	13	GLY	3.2
42	DU	77	THR	3.2
53	B5	62	THR	3.2
12	AL	25	GLU	3.2
34	DM	95	LEU	3.1
36	DO	5	SER	3.1
51	D3	40	ARG	3.1
25	DD	31	ALA	3.1
42	DU	51	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	CA	995	C	3.1
27	DF	74	VAL	3.1
30	BI	9	VAL	3.1
30	DI	139	VAL	3.1
7	AG	7	ILE	3.1
14	CN	52	PRO	3.1
30	DI	26	PRO	3.1
5	CE	157	ARG	3.1
10	CJ	9	ARG	3.1
14	AN	42	TRP	3.1
22	BA	1071	G	3.1
22	BA	2168	G	3.1
22	DA	583	G	3.1
26	DE	143	LEU	3.1
49	D1	21	TYR	3.1
9	CI	121	ALA	3.1
26	DE	179	SER	3.1
36	DO	17	LYS	3.1
41	DT	68	LYS	3.1
50	D2	32	ALA	3.1
1	CA	1236	A	3.1
20	CT	70	ASN	3.1
21	AU	32	VAL	3.1
29	DH	138	VAL	3.1
37	DP	92	VAL	3.1
1	CA	1317	C	3.1
16	CP	3	THR	3.1
40	DS	96	ILE	3.1
27	DF	84	PRO	3.1
30	DI	75	PRO	3.1
5	AE	11	LEU	3.1
14	CN	9	ARG	3.1
14	CN	59	ARG	3.1
26	DE	200	LEU	3.1
20	CT	64	LYS	3.1
42	DU	26	LYS	3.1
28	DG	136	ALA	3.1
29	BH	65	ALA	3.1
30	DI	120	ALA	3.1
22	BA	2133	G	3.1
22	BA	2144	G	3.1
26	DE	178	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
35	DN	29	VAL	3.1
2	AB	155	GLY	3.1
22	BA	2111	U	3.1
22	BA	2113	U	3.1
22	BA	2402	U	3.1
7	CG	72	THR	3.1
24	BC	238	ARG	3.1
44	DW	41	ARG	3.1
9	AI	111	VAL	3.1
14	AN	34	VAL	3.1
14	AN	45	VAL	3.1
28	DG	10	VAL	3.1
30	BI	98	VAL	3.1
22	BA	2140	G	3.1
22	BA	2142	A	3.1
6	CF	91	ARG	3.1
19	CS	3	ARG	3.1
41	DT	42	GLU	3.1
41	DT	73	ARG	3.1
4	AD	8	LYS	3.1
26	DE	153	LEU	3.1
29	BH	71	LYS	3.1
13	CM	61	ALA	3.0
22	BA	1172	C	3.1
27	DF	43	ALA	3.0
28	DG	59	ALA	3.0
51	D3	27	ALA	3.0
53	B5	46	ALA	3.0
7	CG	103	TRP	3.0
14	CN	11	VAL	3.0
27	DF	146	VAL	3.0
51	D3	14	PHE	3.0
53	B5	20	VAL	3.0
33	DL	81	ASP	3.0
42	DU	78	GLY	3.0
9	CI	130	ARG	3.0
21	AU	35	ARG	3.0
50	D2	14	ARG	3.0
16	CP	80	LYS	3.0
39	DR	73	LYS	3.0
1	AA	1492	A	3.0
22	BA	1065	U	3.0

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Mol	Chain	Res	Type	RSRZ
53	B5	182	PRO	3.0
22	BA	2191	A	3.0
9	CI	66	THR	3.0
22	BA	2162	G	3.0
21	CU	15	ALA	3.0
29	BH	56	ALA	3.0
7	CG	69	VAL	3.0
7	CG	151	PHE	3.0
16	CP	39	PHE	3.0
33	DL	89	VAL	3.0
42	DU	36	VAL	3.0
22	DA	1092	C	3.0
8	CH	2	SER	3.0
14	CN	5	SER	3.0
30	BI	135	SER	3.0
29	BH	123	ARG	3.0
2	AB	43	LEU	3.0
7	CG	59	LEU	3.0
50	D2	31	LEU	3.0
7	CG	61	ALA	3.0
22	DA	1057	A	3.0
29	BH	52	ALA	3.0
51	D3	65	ALA	3.0
5	AE	137	VAL	3.0
10	AJ	74	VAL	3.0
29	BH	61	VAL	3.0
22	BA	2138	G	3.0
22	DA	1087	G	3.0
38	DQ	25	TYR	3.0
1	CA	1217	C	3.0
1	CA	1218	C	3.0
10	CJ	82	LYS	3.0
13	CM	24	GLY	3.0
17	CQ	5	ILE	3.0
28	DG	26	ILE	3.0
29	BH	116	ARG	3.0
30	BI	129	ILE	3.0
35	DN	17	ARG	3.0
36	DO	3	LYS	3.0
41	DT	76	ARG	3.0
29	BH	90	LEU	3.0
32	DK	28	SER	3.0

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Mol	Chain	Res	Type	RSRZ
33	DL	106	GLU	3.0
26	DE	68	ALA	3.0
33	DL	15	ALA	3.0
37	DP	95	ALA	3.0
53	B5	123	ALA	3.0
11	AK	113	VAL	3.0
48	D0	25	VAL	3.0
53	B5	124	VAL	3.0
46	DY	54	LYS	3.0
7	CG	4	ARG	3.0
52	D4	16	ILE	3.0
2	CB	13	GLY	3.0
11	AK	43	GLY	3.0
14	CN	4	GLN	3.0
26	DE	3	LEU	3.0
33	DL	53	GLY	3.0
35	DN	65	LEU	3.0
49	D1	11	LEU	3.0
1	CA	211	G	3.0
22	DA	51	G	3.0
7	CG	41	SER	3.0
53	B5	202	PRO	3.0
16	CP	27	ALA	3.0
19	AS	39	THR	3.0
29	DH	79	THR	3.0
13	CM	64	VAL	3.0
21	AU	14	VAL	3.0
42	DU	70	VAL	3.0
51	D3	58	VAL	3.0
1	CA	1364	U	3.0
22	BA	2166	U	3.0
14	CN	3	LYS	2.9
25	DD	8	LYS	2.9
51	D3	23	LYS	2.9
52	D4	9	LYS	2.9
19	CS	55	ARG	2.9
27	BF	80	ARG	2.9
1	AA	78	A	2.9
1	AA	1534	A	2.9
2	CB	67	ILE	2.9
22	BA	2117	A	2.9
22	BA	2171	A	2.9

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Mol	Chain	Res	Type	RSRZ
22	DA	2176	A	2.9
7	AG	59	LEU	2.9
7	CG	50	LEU	2.9
25	DD	144	GLY	2.9
34	DM	23	GLY	2.9
35	DN	105	GLY	2.9
29	BH	66	ASN	2.9
51	D3	2	PRO	2.9
51	D3	28	ASN	2.9
19	CS	4	SER	2.9
53	B5	110	ASP	2.9
53	B5	156	GLU	2.9
22	DA	376	G	2.9
31	DJ	1	MET	2.9
20	CT	38	ALA	2.9
30	BI	44	ALA	2.9
53	B5	90	ALA	2.9
7	CG	18	PHE	2.9
9	CI	127	PHE	2.9
25	DD	26	VAL	2.9
29	DH	130	VAL	2.9
41	DT	55	VAL	2.9
44	DW	23	VAL	2.9
40	DS	9	HIS	2.9
2	AB	131	LYS	2.9
29	BH	112	LYS	2.9
1	CA	4	U	2.9
22	BA	2109	U	2.9
13	CM	9	ILE	2.9
47	DZ	48	ILE	2.9
2	CB	96	TRP	2.9
41	DT	32	LEU	2.9
36	DO	64	TYR	2.9
51	D3	20	GLY	2.9
51	D3	46	PRO	2.9
7	CG	128	ALA	2.9
26	DE	33	VAL	2.9
28	DG	43	VAL	2.9
29	BH	108	VAL	2.9
30	DI	104	ALA	2.9
42	DU	28	VAL	2.9
7	CG	76	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
10	CJ	59	LYS	2.9
19	CS	7	LYS	2.9
9	AI	130	ARG	2.9
1	CA	1026	G	2.9
22	DA	70	G	2.9
18	CR	21	ILE	2.9
30	BI	101	ILE	2.9
22	BA	2122	U	2.9
22	DA	1375	U	2.9
40	DS	19	LEU	2.9
18	AR	20	GLU	2.9
1	CA	978	A	2.9
14	CN	54	ASP	2.9
22	DA	53	A	2.9
41	DT	79	ASP	2.9
9	AI	128	SER	2.9
10	CJ	34	ALA	2.9
10	CJ	84	VAL	2.9
13	AM	5	ALA	2.9
38	DQ	5	LYS	2.9
53	B5	212	SER	2.9
32	BK	35	VAL	2.9
30	BI	38	PHE	2.9
33	DL	66	PHE	2.9
3	CC	192	THR	2.9
19	CS	39	THR	2.9
30	DI	46	THR	2.9
40	DS	99	ARG	2.9
10	CJ	40	ILE	2.9
9	CI	54	LEU	2.9
1	CA	1243	C	2.9
5	AE	104	GLY	2.9
42	DU	84	GLY	2.9
1	CA	94	G	2.9
22	DA	1475	G	2.9
30	BI	93	PRO	2.9
53	B5	163	GLU	2.9
28	DG	6	LYS	2.9
30	BI	100	LYS	2.9
10	AJ	14	ASP	2.9
14	AN	2	ALA	2.9
16	CP	20	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
53	B5	75	VAL	2.9
29	BH	139	PHE	2.9
7	CG	102	ARG	2.9
9	CI	43	THR	2.9
53	B5	35	THR	2.9
4	CD	28	ILE	2.9
10	CJ	73	LEU	2.9
19	CS	13	LEU	2.9
26	DE	118	LEU	2.9
42	DU	103	ILE	2.9
44	DW	59	LEU	2.9
24	DC	209	GLY	2.8
41	BT	90	GLY	2.8
9	CI	5	GLN	2.8
26	DE	94	GLN	2.8
53	B5	108	TRP	2.8
1	AA	1030	U	2.8
1	AA	1539	C	2.8
1	CA	1025	U	2.8
14	CN	12	LYS	2.8
16	CP	17	TYR	2.8
22	BA	2146	C	2.8
49	D1	37	LYS	2.8
1	AA	1018	G	2.8
10	AJ	36	VAL	2.8
22	DA	54	G	2.8
22	DA	1236	G	2.8
22	DA	2112	G	2.8
29	DH	61	VAL	2.8
29	BH	91	PHE	2.8
29	DH	123	ARG	2.8
36	DO	14	ALA	2.8
19	CS	10	PHE	2.8
41	DT	12	ARG	2.8
20	AT	6	SER	2.8
5	AE	103	THR	2.8
15	CO	25	THR	2.8
28	DG	105	LEU	2.8
30	DI	73	THR	2.8
1	CA	994	A	2.8
1	CA	1145	A	2.8
22	DA	504	A	2.8

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Mol	Chain	Res	Type	RSRZ
22	DA	2406	A	2.8
19	CS	68	GLY	2.8
9	CI	126	GLN	2.8
27	DF	27	GLN	2.8
30	DI	113	LYS	2.8
42	DU	43	LYS	2.8
31	DJ	9	GLU	2.8
22	BA	138	U	2.8
22	BA	1060	U	2.8
22	DA	102	U	2.8
7	CG	26	PHE	2.8
22	BA	2129	C	2.8
33	DL	75	ALA	2.8
33	DL	110	VAL	2.8
35	DN	45	ARG	2.8
52	D4	25	VAL	2.8
53	B5	27	ALA	2.8
27	DF	77	PHE	2.8
27	DF	99	PHE	2.8
3	CC	33	LEU	2.8
5	AE	30	ILE	2.8
7	CG	15	ASP	2.8
13	CM	11	ASP	2.8
29	BH	80	ILE	2.8
30	BI	138	LEU	2.8
31	DJ	49	ASP	2.8
39	DR	49	ILE	2.8
41	DT	2	ILE	2.8
41	DT	15	HIS	2.8
19	CS	47	LEU	2.8
1	CA	1020	G	2.8
22	BA	2127	G	2.8
22	DA	2125	G	2.8
1	CA	1363	A	2.8
22	BA	1090	A	2.8
22	BA	1847	A	2.8
22	BA	2108	A	2.8
33	DL	65	GLY	2.8
14	CN	7	LYS	2.8
32	DK	111	LYS	2.8
33	DL	13	LYS	2.8
25	DD	23	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
42	DU	55	PRO	2.8
47	DZ	31	ARG	2.8
51	D3	64	TYR	2.8
9	CI	44	ALA	2.8
13	CM	5	ALA	2.8
22	BA	2106	U	2.8
22	BA	2118	U	2.8
52	D4	22	VAL	2.8
32	DK	112	PHE	2.8
13	CM	69	LEU	2.8
38	DQ	65	ILE	2.8
46	DY	21	LEU	2.8
53	B5	186	LEU	2.8
22	DA	1049	C	2.8
30	DI	121	ASP	2.8
26	DE	131	THR	2.8
27	DF	155	THR	2.8
53	B5	85	LYS	2.8
13	AM	99	GLY	2.8
27	BF	76	GLY	2.8
9	CI	125	PRO	2.8
22	DA	1068	G	2.8
48	D0	8	PRO	2.8
1	CA	1016	A	2.8
22	BA	1067	A	2.8
22	DA	1175	A	2.8
29	BH	114	GLU	2.8
41	DT	10	VAL	2.8
13	AM	63	PHE	2.8
30	DI	8	TYR	2.8
1	CA	209	U	2.8
2	CB	43	LEU	2.8
27	DF	85	ILE	2.8
42	DU	29	LEU	2.8
25	DD	131	ASP	2.8
6	AF	93	LYS	2.8
8	CH	3	MET	2.8
19	CS	21	LYS	2.8
35	DN	20	MET	2.8
45	DX	48	THR	2.8
53	B5	71	LYS	2.8
28	DG	2	SER	2.8

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Mol	Chain	Res	Type	RSRZ
30	BI	89	GLY	2.8
27	DF	80	ARG	2.7
25	DD	155	VAL	2.7
27	BF	74	VAL	2.7
28	DG	11	VAL	2.7
13	CM	40	ALA	2.7
22	BA	2154	A	2.7
27	DF	122	PHE	2.7
30	BI	67	PHE	2.7
43	DV	39	ALA	2.7
9	CI	21	ILE	2.7
17	CQ	25	ILE	2.7
20	CT	66	LEU	2.7
22	DA	2307	G	2.7
46	DY	37	LEU	2.7
7	CG	142	HIS	2.7
22	DA	2109	U	2.7
24	DC	36	LYS	2.7
28	DG	177	LYS	2.7
30	DI	125	MET	2.7
42	DU	4	LYS	2.7
10	CJ	19	ASP	2.7
13	CM	28	THR	2.7
14	AN	55	SER	2.7
35	DN	2	ARG	2.7
46	BY	23	ARG	2.7
22	BA	1914	C	2.7
13	CM	97	VAL	2.7
35	DN	19	ALA	2.7
2	CB	207	ILE	2.7
37	DP	84	ILE	2.7
46	DY	41	HIS	2.7
11	AK	14	LYS	2.7
26	DE	95	LYS	2.7
51	D3	25	LYS	2.7
1	CA	1240	U	2.7
22	DA	107	G	2.7
9	CI	31	ASN	2.7
5	CE	109	GLY	2.7
27	DF	41	GLY	2.7
26	DE	177	PRO	2.7
29	DH	32	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
30	BI	75	PRO	2.7
31	DJ	37	ARG	2.7
10	CJ	99	GLN	2.7
9	CI	104	VAL	2.7
1	CA	1031	C	2.7
7	CG	150	ALA	2.7
13	CM	4	ILE	2.7
26	DE	135	ALA	2.7
27	DF	91	LEU	2.7
30	BI	120	ALA	2.7
33	DL	103	ILE	2.7
38	DQ	38	ALA	2.7
51	D3	37	ALA	2.7
2	AB	11	LYS	2.7
2	CB	45	LYS	2.7
7	CG	137	LYS	2.7
9	CI	129	LYS	2.7
24	DC	265	LYS	2.7
41	DT	40	LYS	2.7
42	DU	33	LYS	2.7
53	B5	37	LYS	2.7
30	BI	117	MET	2.7
1	CA	1224	U	2.7
13	AM	105	ASN	2.7
19	AS	33	THR	2.7
22	DA	1065	U	2.7
22	DA	1325	U	2.7
13	CM	112	PRO	2.7
25	DD	77	ARG	2.7
33	DL	34	GLY	2.7
42	DU	90	GLY	2.7
46	DY	55	THR	2.7
53	B5	107	GLY	2.7
53	B5	208	THR	2.7
1	CA	1032	G	2.7
1	CA	1241	G	2.7
9	CI	32	GLN	2.7
22	DA	329	G	2.7
22	DA	1311	G	2.7
30	DI	102	SER	2.7
19	CS	58	VAL	2.7
7	AG	12	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
14	CN	46	LEU	2.7
39	DR	27	ILE	2.7
41	DT	50	LEU	2.7
53	B5	87	ALA	2.7
53	B5	162	ILE	2.7
53	B5	197	LEU	2.7
30	DI	115	ALA	2.7
53	B5	196	ALA	2.7
19	CS	18	LYS	2.7
30	BI	92	LYS	2.7
30	DI	97	LYS	2.7
53	B5	83	LYS	2.7
26	DE	199	MET	2.7
13	CM	12	HIS	2.7
22	BA	2143	C	2.7
22	BA	2165	C	2.7
10	CJ	45	ARG	2.7
10	CJ	72	ARG	2.7
14	CN	63	ARG	2.7
46	DY	47	ARG	2.7
12	CL	92	GLY	2.7
51	D3	17	THR	2.7
22	BA	1089	A	2.7
22	BA	2181	U	2.7
22	DA	224	U	2.7
22	DA	1058	U	2.7
36	DO	93	ASP	2.7
5	CE	123	VAL	2.7
26	DE	77	ILE	2.6
29	BH	58	LEU	2.7
29	DH	75	LEU	2.7
30	DI	92	LYS	2.6
36	DO	58	ILE	2.6
36	DO	87	ILE	2.6
47	DZ	32	ILE	2.6
10	CJ	49	PHE	2.6
30	BI	77	ALA	2.6
1	CA	1331	G	2.6
22	BA	549	G	2.6
22	DA	2120	G	2.6
27	DF	130	MET	2.6
45	DX	20	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
15	AO	89	ARG	2.6
21	CU	47	ARG	2.6
1	CA	207	C	2.6
13	CM	26	GLY	2.6
30	DI	32	GLY	2.6
13	CM	20	THR	2.6
46	DY	16	THR	2.6
4	AD	152	GLN	2.6
22	DA	29	U	2.6
22	DA	2402	U	2.6
1	AA	1493	A	2.6
14	CN	82	ILE	2.6
19	AS	49	ILE	2.6
26	DE	74	LYS	2.6
29	DH	58	LEU	2.6
29	DH	141	LYS	2.6
30	BI	3	LYS	2.6
42	BU	52	LEU	2.6
52	D4	20	ASP	2.6
38	DQ	74	ILE	2.6
7	CG	54	SER	2.6
30	DI	41	ALA	2.6
30	DI	44	ALA	2.6
41	DT	70	HIS	2.6
13	CM	98	ARG	2.6
28	DG	170	ARG	2.6
47	DZ	11	ARG	2.6
27	DF	29	PRO	2.6
53	B5	134	PRO	2.6
7	CG	87	VAL	2.6
13	CM	95	LEU	2.6
22	DA	76	C	2.6
37	DP	115	ASN	2.6
48	D0	7	LYS	2.6
8	AH	76	GLN	2.6
19	CS	24	GLU	2.6
29	BH	78	VAL	2.6
27	DF	137	ILE	2.6
36	DO	98	GLN	2.6
29	BH	86	ASP	2.6
7	CG	65	ALA	2.6
10	AJ	34	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
12	AL	23	ALA	2.6
25	DD	209	ALA	2.6
27	DF	20	PHE	2.6
28	DG	52	PHE	2.6
29	BH	106	ALA	2.6
30	BI	84	ALA	2.6
1	CA	1219	A	2.6
20	CT	6	SER	2.6
22	DA	1214	A	2.6
22	DA	1237	A	2.6
19	CS	14	HIS	2.6
38	DQ	28	ARG	2.6
50	D2	21	ARG	2.6
43	DV	57	TYR	2.6
30	DI	52	GLY	2.6
29	DH	83	LYS	2.6
31	DJ	111	LYS	2.6
2	AB	135	LEU	2.6
7	CG	124	LEU	2.6
10	AJ	77	VAL	2.6
13	CM	104	THR	2.6
39	DR	22	LEU	2.6
2	AB	164	ILE	2.6
41	BT	2	ILE	2.6
46	BY	11	VAL	2.6
26	DE	104	ALA	2.6
29	BH	74	ALA	2.6
36	DO	23	ALA	2.6
50	D2	36	ALA	2.6
1	CA	1322	C	2.6
22	DA	1061	U	2.6
1	CA	1019	A	2.6
22	BA	1088	A	2.6
2	AB	213	TYR	2.6
4	AD	22	LYS	2.6
7	CG	85	TYR	2.6
27	DF	83	TYR	2.6
30	DI	45	LYS	2.6
29	BH	88	GLY	2.6
30	DI	131	GLY	2.6
25	DD	79	LEU	2.6
36	DO	18	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
2	AB	9	MET	2.6
2	CB	164	ILE	2.6
9	AI	21	ILE	2.6
27	DF	40	VAL	2.6
50	D2	1	MET	2.6
53	B5	95	VAL	2.6
9	AI	44	ALA	2.6
12	CL	26	ALA	2.6
25	DD	132	ALA	2.6
1	CA	1018	G	2.5
22	BA	1062	G	2.5
22	BA	2110	G	2.5
22	DA	327	G	2.5
22	DA	409	G	2.5
22	DA	2116	G	2.5
22	DA	2127	G	2.5
1	CA	1321	U	2.5
9	CI	18	ARG	2.5
22	BA	884	U	2.5
22	DA	1094	U	2.5
25	DD	59	ARG	2.5
27	DF	125	ARG	2.5
29	DH	128	HIS	2.5
47	DZ	30	ARG	2.5
22	BA	1100	C	2.5
22	BA	2153	C	2.5
27	DF	129	SER	2.5
29	DH	131	SER	2.5
40	DS	81	SER	2.5
9	CI	120	LYS	2.5
13	CM	44	LYS	2.5
36	DO	63	LYS	2.5
37	DP	111	LYS	2.5
51	D3	19	LYS	2.5
22	DA	1077	A	2.5
13	CM	99	GLY	2.5
14	AN	27	LEU	2.5
29	BH	95	GLY	2.5
36	DO	106	LEU	2.5
41	DT	61	LEU	2.5
39	DR	72	VAL	2.5
42	DU	35	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
53	B5	219	MET	2.5
14	CN	66	GLN	2.5
21	CU	36	GLU	2.5
29	BH	133	GLN	2.5
30	BI	71	THR	2.5
21	CU	37	PHE	2.5
30	BI	110	ALA	2.5
26	DE	67	ARG	2.5
30	DI	116	ASP	2.5
36	DO	2	ASP	2.5
39	DR	80	ARG	2.5
1	CA	1017	U	2.5
19	CS	17	LYS	2.5
46	DY	40	SER	2.5
52	D4	8	LYS	2.5
22	DA	215	G	2.5
1	CA	330	C	2.5
30	BI	99	GLY	2.5
32	DK	68	GLY	2.5
33	DL	57	LEU	2.5
53	B5	144	GLY	2.5
3	CC	94	ILE	2.5
19	CS	67	VAL	2.5
29	BH	138	VAL	2.5
29	BH	147	VAL	2.5
29	DH	143	ILE	2.5
33	DL	100	ILE	2.5
53	B5	101	ILE	2.5
33	BL	115	GLU	2.5
29	BH	84	ALA	2.5
30	DI	15	ALA	2.5
30	DI	18	ALA	2.5
35	DN	111	ALA	2.5
46	DY	61	ALA	2.5
53	B5	143	ALA	2.5
9	CI	124	ARG	2.5
36	DO	10	ARG	2.5
44	DW	39	ARG	2.5
45	DX	11	ARG	2.5
44	DW	62	LYS	2.5
50	D2	2	LYS	2.5
4	AD	38	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
29	BH	54	LEU	2.5
24	BC	235	GLY	2.5
53	B5	100	ILE	2.5
24	DC	216	VAL	2.5
41	DT	80	TRP	2.5
22	BA	1924	C	2.5
22	DA	343	C	2.5
1	CA	1024	G	2.5
22	BA	2128	G	2.5
22	DA	266	G	2.5
22	DA	619	G	2.5
19	CS	41	PHE	2.5
33	DL	64	PHE	2.5
13	AM	35	ALA	2.5
14	CN	29	ALA	2.5
19	CS	75	ALA	2.5
26	DE	128	ALA	2.5
35	DN	18	GLN	2.5
48	D0	56	ALA	2.5
1	CA	977	A	2.5
22	DA	311	A	2.5
22	DA	505	A	2.5
30	DI	95	LYS	2.5
36	DO	56	LYS	2.5
41	DT	88	LYS	2.5
20	AT	86	LEU	2.5
26	DE	164	LEU	2.5
33	DL	3	LEU	2.5
13	CM	96	PRO	2.5
41	BT	1	MET	2.5
42	DU	48	PRO	2.5
45	DX	31	PRO	2.5
46	DY	30	MET	2.5
26	DE	70	SER	2.5
1	AA	842	U	2.5
2	CB	65	GLY	2.5
30	DI	66	SER	2.5
48	D0	18	SER	2.5
22	BA	1058	U	2.5
2	CB	14	VAL	2.5
29	DH	121	VAL	2.5
3	AC	168	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
10	CJ	47	GLU	2.5
36	DO	97	PHE	2.5
42	DU	85	PHE	2.5
2	CB	139	ARG	2.5
14	CN	36	ALA	2.5
19	CS	78	ARG	2.5
30	BI	41	ALA	2.5
38	DQ	33	ARG	2.5
42	DU	66	GLN	2.5
2	AB	132	LYS	2.5
7	AG	25	LYS	2.5
22	DA	885	C	2.5
22	DA	1076	C	2.5
50	D2	43	THR	2.5
29	DH	35	LYS	2.5
32	DK	66	LYS	2.5
50	D2	37	LYS	2.5
22	BA	880	G	2.5
22	BA	2116	G	2.5
22	DA	277	G	2.5
22	DA	2123	G	2.5
1	CA	1227	A	2.5
13	CM	14	HIS	2.5
22	BA	1080	A	2.5
22	BA	2163	A	2.5
22	DA	477	A	2.5
22	DA	1205	A	2.5
22	DA	1213	A	2.5
53	B5	45	HIS	2.5
24	DC	45	ASN	2.5
35	DN	107	ASN	2.5
7	CG	30	LEU	2.4
29	DH	54	LEU	2.4
30	BI	17	MET	2.4
41	DT	87	LEU	2.4
47	DZ	24	LEU	2.4
50	D2	10	LEU	2.4
2	AB	67	ILE	2.4
19	CS	40	ILE	2.4
20	CT	57	ILE	2.4
25	DD	27	ILE	2.4
31	DJ	46	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
53	B5	194	ILE	2.4
3	CC	158	GLY	2.4
16	CP	10	GLY	2.4
4	AD	23	SER	2.4
10	CJ	57	VAL	2.4
14	CN	32	SER	2.4
24	DC	172	VAL	2.4
27	DF	39	GLY	2.4
35	DN	101	GLY	2.4
50	D2	45	SER	2.4
1	AA	1537	U	2.4
22	BA	2167	U	2.4
22	DA	2213	U	2.4
3	CC	167	TRP	2.4
14	CN	42	TRP	2.4
19	AS	55	ARG	2.4
24	BC	240	PHE	2.4
42	DU	60	GLU	2.4
3	CC	45	LYS	2.4
13	CM	36	ALA	2.4
26	DE	201	ALA	2.4
27	DF	75	ALA	2.4
29	DH	39	ALA	2.4
30	BI	72	LYS	2.4
35	DN	40	LYS	2.4
49	D1	10	LYS	2.4
50	D2	25	LYS	2.4
51	D3	60	ALA	2.4
53	B5	22	THR	2.4
22	DA	57	C	2.4
22	DA	509	C	2.4
9	CI	4	ASN	2.4
9	CI	63	LEU	2.4
22	DA	332	A	2.4
22	DA	1608	A	2.4
27	DF	60	ILE	2.4
53	B5	104	ILE	2.4
26	DE	103	GLY	2.4
27	DF	13	VAL	2.4
41	DT	47	VAL	2.4
18	AR	73	ARG	2.4
26	DE	55	SER	2.4

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Mol	Chain	Res	Type	RSRZ
36	DO	15	ARG	2.4
38	DQ	6	ARG	2.4
38	DQ	87	SER	2.4
40	DS	11	ARG	2.4
45	DX	18	ARG	2.4
48	D0	52	ARG	2.4
53	B5	180	SER	2.4
7	CG	114	LYS	2.4
12	CL	44	LYS	2.4
13	AM	31	LYS	2.4
22	DA	846	U	2.4
35	DN	102	PHE	2.4
2	CB	209	ALA	2.4
7	CG	46	ALA	2.4
10	CJ	61	ALA	2.4
27	DF	55	ALA	2.4
29	BH	100	ALA	2.4
3	CC	44	THR	2.4
19	AS	77	THR	2.4
35	DN	3	HIS	2.4
7	CG	120	LEU	2.4
33	DL	82	LEU	2.4
35	DN	10	LEU	2.4
45	DX	56	MET	2.4
1	CA	1132	C	2.4
22	DA	1064	C	2.4
30	BI	20	PRO	2.4
13	CM	94	GLY	2.4
25	DD	76	GLY	2.4
30	DI	85	GLY	2.4
32	DK	81	GLY	2.4
33	DL	16	GLY	2.4
53	B5	207	GLY	2.4
1	CA	1021	A	2.4
4	CD	151	LYS	2.4
42	DU	17	LYS	2.4
20	CT	14	SER	2.4
22	DA	180	G	2.4
22	DA	356	G	2.4
22	DA	974	G	2.4
22	DA	1063	G	2.4
22	DA	2107	G	2.4

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Mol	Chain	Res	Type	RSRZ
53	B5	55	SER	2.4
13	CM	106	ALA	2.4
17	AQ	82	ALA	2.4
39	DR	36	ALA	2.4
30	DI	105	GLN	2.4
38	DQ	44	GLN	2.4
27	DF	38	MET	2.4
53	B5	109	MET	2.4
46	DY	42	LEU	2.4
13	CM	39	ILE	2.4
35	DN	113	ILE	2.4
19	AS	30	PRO	2.4
53	B5	175	PRO	2.4
7	CG	132	GLY	2.4
7	CG	141	VAL	2.4
2	AB	28	LYS	2.4
12	CL	15	LYS	2.4
24	DC	41	GLY	2.4
24	DC	47	GLY	2.4
29	BH	3	VAL	2.4
30	BI	57	VAL	2.4
37	DP	73	VAL	2.4
39	DR	96	VAL	2.4
27	DF	161	LYS	2.4
42	DU	47	LYS	2.4
51	D3	3	LYS	2.4
53	B5	91	GLY	2.4
13	CM	109	ARG	2.4
22	DA	508	A	2.4
26	DE	158	PHE	2.4
26	DE	183	PHE	2.4
13	CM	35	ALA	2.4
14	AN	29	ALA	2.4
14	CN	44	ALA	2.4
41	DT	45	ALA	2.4
42	DU	75	ALA	2.4
46	DY	33	ALA	2.4
30	BI	66	SER	2.4
33	DL	12	SER	2.4
26	DE	78	TRP	2.4
1	AA	86	G	2.4
1	CA	1307	U	2.4

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Mol	Chain	Res	Type	RSRZ
18	AR	23	TYR	2.4
19	CS	48	THR	2.4
22	BA	2157	G	2.4
22	DA	308	G	2.4
22	DA	1066	U	2.4
22	DA	1078	U	2.4
22	DA	2382	G	2.4
29	DH	124	THR	2.4
30	DI	71	THR	2.4
30	DI	117	MET	2.4
36	DO	26	LEU	2.4
48	D0	19	HIS	2.4
48	D0	39	LEU	2.4
13	AM	4	ILE	2.4
30	BI	109	ILE	2.4
36	DO	35	ILE	2.4
10	AJ	39	PRO	2.4
2	CB	37	LYS	2.3
13	AM	25	VAL	2.3
17	CQ	23	VAL	2.3
2	AB	202	GLY	2.3
13	CM	87	ARG	2.3
19	AS	3	ARG	2.3
28	DG	162	VAL	2.3
45	DX	77	LYS	2.3
19	CS	8	GLY	2.3
13	CM	85	CYS	2.3
8	CH	130	ALA	2.3
26	DE	86	ALA	2.3
29	BH	55	GLU	2.3
29	BH	64	ALA	2.3
29	BH	140	ALA	2.3
35	DN	55	ALA	2.3
15	CO	80	GLN	2.3
22	DA	357	C	2.3
1	CA	1318	A	2.3
7	CG	77	SER	2.3
10	CJ	54	SER	2.3
14	AN	56	SER	2.3
22	BA	2126	A	2.3
22	BA	2170	A	2.3
22	DA	429	A	2.3

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Mol	Chain	Res	Type	RSRZ
24	DC	248	TRP	2.3
2	CB	138	THR	2.3
3	AC	21	THR	2.3
7	CG	44	TYR	2.3
18	AR	74	HIS	2.3
19	CS	5	LEU	2.3
28	DG	58	TYR	2.3
29	DH	125	THR	2.3
33	DL	118	THR	2.3
48	D0	42	HIS	2.3
49	D1	19	HIS	2.3
51	D3	24	HIS	2.3
10	CJ	8	ILE	2.3
10	CJ	25	ILE	2.3
29	DH	72	ILE	2.3
36	DO	40	ILE	2.3
41	DT	30	ILE	2.3
53	B5	157	ILE	2.3
9	CI	100	LYS	2.3
20	AT	5	LYS	2.3
35	DN	35	LYS	2.3
38	DQ	41	LYS	2.3
1	CA	971	G	2.3
1	CA	1002	G	2.3
2	AB	187	VAL	2.3
3	CC	91	VAL	2.3
3	CC	195	VAL	2.3
7	AG	4	ARG	2.3
22	BA	277	G	2.3
22	DA	2308	G	2.3
40	DS	20	VAL	2.3
41	DT	62	VAL	2.3
42	BU	49	VAL	2.3
42	DU	93	VAL	2.3
42	DU	57	GLY	2.3
2	AB	16	PHE	2.3
2	CB	88	ASP	2.3
3	CC	30	ALA	2.3
29	DH	65	ALA	2.3
29	DH	140	ALA	2.3
38	DQ	27	ALA	2.3
46	DY	59	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
53	B5	198	GLU	2.3
30	BI	136	MET	2.3
38	DQ	71	GLN	2.3
29	DH	12	LEU	2.3
30	BI	106	LEU	2.3
3	AC	167	TRP	2.3
1	AA	1031	C	2.3
1	CA	979	C	2.3
12	CL	40	THR	2.3
13	CM	102	THR	2.3
22	DA	32	C	2.3
1	AA	1441	A	2.3
20	CT	67	ILE	2.3
27	DF	90	THR	2.3
33	DL	67	THR	2.3
22	DA	2119	A	2.3
49	D1	5	ILE	2.3
3	CC	79	LYS	2.3
40	DS	6	LYS	2.3
40	DS	98	LYS	2.3
1	AA	4	U	2.3
1	CA	950	U	2.3
1	CA	1183	U	2.3
9	CI	23	PRO	2.3
21	AU	17	ARG	2.3
22	DA	328	U	2.3
53	B5	161	ARG	2.3
2	AB	221	VAL	2.3
3	CC	52	VAL	2.3
30	BI	58	VAL	2.3
32	BK	122	VAL	2.3
26	DE	64	GLY	2.3
36	DO	96	GLY	2.3
35	DN	11	ASN	2.3
46	DY	26	PHE	2.3
1	AA	79	G	2.3
1	CA	212	G	2.3
1	CA	1047	G	2.3
22	BA	879	G	2.3
22	DA	117	G	2.3
22	DA	333	G	2.3
22	DA	476	G	2.3

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Mol	Chain	Res	Type	RSRZ
24	DC	211	ALA	2.3
29	BH	105	ALA	2.3
39	DR	103	ALA	2.3
53	B5	187	ALA	2.3
14	CN	6	MET	2.3
43	DV	43	ASP	2.3
6	CF	39	LEU	2.3
30	DI	30	GLN	2.3
2	AB	41	ILE	2.3
2	CB	152	LYS	2.3
7	AG	37	SER	2.3
24	DC	64	ILE	2.3
26	DE	166	LYS	2.3
30	BI	97	LYS	2.3
42	DU	91	LYS	2.3
51	D3	4	ILE	2.3
53	B5	173	HIS	2.3
19	AS	32	ARG	2.3
27	DF	22	TYR	2.3
39	DR	13	ARG	2.3
39	DR	78	ARG	2.3
50	D2	19	ARG	2.3
1	CA	1001	C	2.3
14	CN	45	VAL	2.3
22	BA	1057	A	2.3
22	BA	2119	A	2.3
22	BA	2306	C	2.3
22	DA	267	C	2.3
22	DA	391	A	2.3
22	DA	2150	C	2.3
23	DB	60	C	2.3
25	DD	9	VAL	2.3
30	BI	139	VAL	2.3
31	DJ	48	VAL	2.3
41	DT	63	VAL	2.3
49	D1	41	PRO	2.3
53	B5	177	GLY	2.3
29	DH	47	PHE	2.3
40	DS	40	ASN	2.3
45	DX	46	PHE	2.3
50	D2	13	ASN	2.3
5	CE	152	MET	2.3

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Mol	Chain	Res	Type	RSRZ
19	CS	66	MET	2.3
21	AU	30	ALA	2.3
29	DH	111	ALA	2.3
33	DL	83	ALA	2.3
53	B5	25	GLU	2.3
53	B5	174	ALA	2.3
2	AB	10	LEU	2.3
34	DM	2	LEU	2.3
43	DV	38	LEU	2.3
4	AD	156	LYS	2.3
11	AK	75	LYS	2.3
29	DH	41	LYS	2.3
30	DI	72	LYS	2.3
47	DZ	19	LYS	2.3
53	B5	80	LYS	2.3
1	AA	844	G	2.3
1	CA	976	G	2.3
3	CC	196	ILE	2.3
18	CR	74	HIS	2.3
22	DA	48	G	2.3
30	DI	122	ILE	2.3
42	DU	72	ILE	2.3
7	CG	57	SER	2.3
11	AK	13	ARG	2.3
29	BH	136	SER	2.3
34	DM	40	ARG	2.3
36	DO	30	ARG	2.3
39	DR	19	THR	2.3
43	DV	3	THR	2.3
53	B5	222	SER	2.3
33	DL	8	PRO	2.3
38	DQ	45	TYR	2.3
7	AG	69	VAL	2.3
19	CS	23	VAL	2.3
35	DN	47	VAL	2.3
39	DR	20	VAL	2.3
40	DS	47	VAL	2.3
52	D4	17	VAL	2.3
53	B5	183	PRO	2.3
3	AC	2	GLY	2.3
3	CC	9	GLY	2.3
5	CE	158	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
49	D1	18	GLY	2.3
22	BA	2131	U	2.3
22	DA	72	U	2.3
22	DA	234	U	2.3
22	DA	354	A	2.2
22	DA	393	C	2.2
22	DA	412	A	2.2
24	DC	240	PHE	2.2
3	CC	48	ALA	2.2
29	BH	73	ASN	2.2
29	DH	81	ALA	2.2
36	DO	46	GLU	2.2
42	DU	2	ALA	2.2
44	DW	17	GLU	2.2
12	AL	24	LEU	2.2
13	CM	80	LEU	2.2
27	DF	50	LEU	2.2
28	DG	27	LYS	2.2
41	DT	49	LYS	2.2
43	DV	87	GLN	2.2
46	DY	36	GLN	2.2
28	DG	166	ASP	2.2
34	DM	70	ASP	2.2
10	CJ	18	ILE	2.2
4	AD	63	ARG	2.2
40	DS	100	THR	2.2
27	DF	73	SER	2.2
28	DG	92	VAL	2.2
29	BH	134	VAL	2.2
46	DY	11	VAL	2.2
48	D0	54	VAL	2.2
31	DJ	74	TYR	2.2
1	CA	993	G	2.2
35	DN	7	GLY	2.2
9	AI	46	MET	2.2
35	DN	21	PHE	2.2
1	CA	1126	U	2.2
22	BA	1061	U	2.2
22	DA	2149	U	2.2
22	DA	2189	U	2.2
16	CP	11	ALA	2.2
20	AT	7	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
37	DP	49	ALA	2.2
15	AO	57	LEU	2.2
22	BA	654	A	2.2
27	DF	36	LEU	2.2
29	DH	15	LEU	2.2
32	DK	89	ASN	2.2
42	DU	79	LYS	2.2
46	DY	14	LEU	2.2
46	DY	57	LEU	2.2
22	DA	1278	C	2.2
4	CD	36	GLN	2.2
9	CI	72	ILE	2.2
27	DF	111	ILE	2.2
30	BI	122	ILE	2.2
36	DO	19	GLN	2.2
24	DC	214	ARG	2.2
25	DD	200	ASP	2.2
33	DL	2	ARG	2.2
36	DO	9	ARG	2.2
53	B5	200	HIS	2.2
9	AI	19	VAL	2.2
13	AM	104	THR	2.2
21	AU	53	VAL	2.2
32	DK	65	THR	2.2
34	DM	24	THR	2.2
40	DS	37	THR	2.2
14	AN	5	SER	2.2
19	CS	38	SER	2.2
29	DH	82	SER	2.2
30	DI	21	SER	2.2
35	DN	6	SER	2.2
2	CB	149	GLY	2.2
9	AI	26	GLY	2.2
20	CT	65	GLY	2.2
24	DC	249	GLY	2.2
31	DJ	118	MET	2.2
2	CB	83	ALA	2.2
7	CG	22	LEU	2.2
7	CG	149	LYS	2.2
13	CM	19	LEU	2.2
16	AP	76	LYS	2.2
16	AP	80	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
27	BF	42	GLU	2.2
27	DF	107	ALA	2.2
36	DO	70	ALA	2.2
39	DR	24	LYS	2.2
40	DS	73	LYS	2.2
21	CU	8	GLU	2.2
22	DA	1091	G	2.2
22	DA	1587	G	2.2
22	DA	2115	G	2.2
22	DA	2410	G	2.2
23	DB	72	G	2.2
33	BL	106	GLU	2.2
46	BY	63	ALA	2.2
22	BA	2189	U	2.2
22	DA	2903	U	2.2
27	DF	30	ARG	2.2
32	DK	2	ILE	2.2
45	DX	64	ILE	2.2
1	CA	1360	A	2.2
22	DA	428	A	2.2
22	DA	626	A	2.2
22	DA	892	A	2.2
22	BA	1606	C	2.2
27	DF	113	ASP	2.2
53	B5	106	ASP	2.2
7	CG	135	VAL	2.2
9	CI	19	VAL	2.2
9	CI	29	VAL	2.2
10	CJ	51	VAL	2.2
2	AB	130	THR	2.2
3	AC	193	TYR	2.2
9	CI	90	TYR	2.2
28	DG	74	SER	2.2
28	DG	157	TYR	2.2
42	DU	32	GLY	2.2
51	D3	18	GLY	2.2
53	B5	126	SER	2.2
53	B5	133	GLY	2.2
2	AB	50	PHE	2.2
7	CG	110	LYS	2.2
27	BF	69	LYS	2.2
31	DJ	39	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
2	CB	57	LEU	2.2
11	AK	82	LEU	2.2
25	DD	40	LEU	2.2
7	CG	152	ALA	2.2
21	AU	39	GLU	2.2
28	DG	32	GLU	2.2
3	CC	207	ILE	2.2
10	CJ	6	ILE	2.2
29	DH	27	ARG	2.2
31	DJ	142	ILE	2.2
1	CA	1286	U	2.2
15	CO	62	GLN	2.2
22	DA	2690	U	2.2
51	D3	42	ARG	2.2
27	DF	135	GLN	2.2
22	DA	914	G	2.2
22	DA	1339	G	2.2
22	DA	1653	G	2.2
22	DA	2405	G	2.2
29	BH	135	HIS	2.2
1	AA	77	A	2.2
1	CA	532	A	2.2
7	CG	88	PRO	2.2
10	CJ	98	VAL	2.2
13	CM	65	VAL	2.2
22	DA	222	A	2.2
22	DA	2062	A	2.2
24	DC	250	VAL	2.2
28	DG	137	ASP	2.2
35	DN	39	PRO	2.2
35	DN	116	VAL	2.2
36	DO	27	VAL	2.2
41	DT	67	VAL	2.2
44	DW	38	VAL	2.2
49	D1	47	VAL	2.2
53	B5	39	ASP	2.2
22	DA	236	C	2.2
22	DA	565	C	2.2
22	DA	1306	C	2.2
10	CJ	69	THR	2.2
11	AK	111	THR	2.2
49	D1	22	THR	2.2

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Mol	Chain	Res	Type	RSRZ
5	AE	102	GLY	2.2
17	CQ	16	LYS	2.2
30	BI	16	GLY	2.2
35	DN	99	LYS	2.2
37	DP	94	LYS	2.2
37	DP	96	LYS	2.2
41	DT	81	LYS	2.2
53	B5	201	LYS	2.2
30	BI	62	TYR	2.2
31	DJ	119	PHE	2.2
53	B5	94	TYR	2.2
53	B5	164	PHE	2.2
4	AD	21	LEU	2.2
13	CM	48	LEU	2.2
14	CN	74	LEU	2.2
34	DM	124	LEU	2.2
43	DV	42	LEU	2.2
51	D3	29	LEU	2.2
2	AB	83	ALA	2.2
7	CG	40	GLU	2.2
7	CG	123	GLU	2.2
14	CN	26	GLU	2.2
21	CU	52	ALA	2.2
2	CB	60	ILE	2.1
13	AM	101	ARG	2.1
24	DC	48	ARG	2.1
32	DK	98	ARG	2.1
34	DM	96	ILE	2.1
40	DS	85	ILE	2.1
22	DA	113	U	2.1
22	DA	235	U	2.1
21	CU	41	PRO	2.1
26	DE	186	VAL	2.1
27	DF	176	PRO	2.1
29	DH	110	VAL	2.1
29	DH	134	VAL	2.1
42	DU	49	VAL	2.1
14	CN	28	LYS	2.1
21	AU	54	LYS	2.1
1	CA	1022	A	2.1
22	BA	613	A	2.1
22	BA	892	A	2.1

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Mol	Chain	Res	Type	RSRZ
22	BA	1068	G	2.1
22	BA	1179	G	2.1
22	DA	118	A	2.1
22	DA	124	G	2.1
22	DA	127	A	2.1
22	DA	330	A	2.1
22	DA	410	G	2.1
22	DA	1321	A	2.1
29	DH	126	GLY	2.1
30	BI	137	GLY	2.1
48	D0	9	THR	2.1
1	AA	995	C	2.1
1	CA	1234	C	2.1
7	AG	26	PHE	2.1
9	CI	87	LEU	2.1
9	CI	118	LEU	2.1
19	AS	74	PHE	2.1
22	DA	33	C	2.1
22	DA	2165	C	2.1
22	DA	2666	C	2.1
23	DB	31	C	2.1
26	DE	112	LEU	2.1
29	DH	132	PHE	2.1
53	B5	181	PHE	2.1
2	CB	134	ALA	2.1
4	CD	23	SER	2.1
9	AI	108	ALA	2.1
27	DF	162	SER	2.1
29	BH	49	ALA	2.1
31	DJ	95	ARG	2.1
36	DO	7	ARG	2.1
52	D4	36	ARG	2.1
7	CG	104	ILE	2.1
13	AM	45	ILE	2.1
28	DG	19	ILE	2.1
31	DJ	103	ILE	2.1
53	B5	150	ILE	2.1
27	DF	21	ASN	2.1
7	AG	80	VAL	2.1
22	DA	392	U	2.1
26	DE	28	VAL	2.1
28	DG	102	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
29	BH	144	VAL	2.1
31	DJ	8	PRO	2.1
36	DO	54	VAL	2.1
41	DT	58	VAL	2.1
46	DY	46	VAL	2.1
35	DN	1	MET	2.1
3	AC	80	LYS	2.1
5	CE	23	LYS	2.1
8	CH	56	LYS	2.1
27	DF	64	LYS	2.1
30	DI	51	LYS	2.1
10	CJ	50	THR	2.1
27	DF	68	THR	2.1
30	BI	68	THR	2.1
30	DI	126	THR	2.1
33	DL	114	GLY	2.1
44	BW	10	THR	2.1
45	DX	14	THR	2.1
48	D0	26	THR	2.1
2	CB	90	PHE	2.1
10	AJ	90	LEU	2.1
18	AR	68	LEU	2.1
21	AU	19	PHE	2.1
26	DE	133	LEU	2.1
27	DF	100	PHE	2.1
27	DF	152	LEU	2.1
29	DH	139	PHE	2.1
47	DZ	17	LEU	2.1
5	CE	75	ALA	2.1
18	CR	51	TYR	2.1
22	DA	2860	A	2.1
26	DE	34	ALA	2.1
27	DF	102	ARG	2.1
41	BT	69	ARG	2.1
53	B5	130	ARG	2.1
53	B5	171	ALA	2.1
9	CI	65	ILE	2.1
22	BA	141	G	2.1
22	DA	1407	G	2.1
22	BA	1102	C	2.1
22	DA	335	C	2.1
22	DA	2310	C	2.1

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Mol	Chain	Res	Type	RSRZ
34	DM	27	SER	2.1
15	AO	80	GLN	2.1
42	BU	54	GLN	2.1
9	AI	55	VAL	2.1
7	CG	16	PRO	2.1
10	CJ	11	LYS	2.1
13	AM	114	LYS	2.1
27	DF	47	LYS	2.1
28	DG	23	VAL	2.1
29	BH	8	LYS	2.1
29	DH	22	LYS	2.1
38	DQ	34	VAL	2.1
40	DS	82	MET	2.1
42	DU	21	LYS	2.1
44	DW	78	LYS	2.1
50	D2	30	VAL	2.1
22	BA	2151	U	2.1
3	CC	29	PHE	2.1
12	AL	109	ASP	2.1
44	DW	42	GLY	2.1
53	B5	70	GLY	2.1
25	DD	68	PHE	2.1
30	BI	132	THR	2.1
33	DL	50	PHE	2.1
6	AF	79	ARG	2.1
21	AU	34	ARG	2.1
37	DP	93	ARG	2.1
7	CG	117	ALA	2.1
25	DD	196	ALA	2.1
28	DG	77	ILE	2.1
35	DN	41	ALA	2.1
9	CI	38	TYR	2.1
29	BH	137	GLU	2.1
13	AM	46	SER	2.1
22	DA	866	A	2.1
23	DB	45	A	2.1
29	DH	113	SER	2.1
39	DR	91	GLN	2.1
1	CA	102	G	2.1
1	CA	1359	C	2.1
3	CC	66	VAL	2.1
10	CJ	46	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
21	CU	54	LYS	2.1
24	DC	232	HIS	2.1
22	BA	2190	G	2.1
22	DA	45	G	2.1
22	DA	115	C	2.1
22	DA	336	C	2.1
26	DE	98	LYS	2.1
28	DG	45	HIS	2.1
22	DA	506	G	2.1
22	DA	1099	G	2.1
22	DA	1212	G	2.1
22	DA	1271	G	2.1
22	DA	1382	G	2.1
23	DB	41	G	2.1
25	DD	5	VAL	2.1
29	DH	118	PRO	2.1
30	BI	74	PRO	2.1
25	DD	185	ASN	2.1
29	DH	73	ASN	2.1
29	DH	119	ASN	2.1
45	DX	17	ASN	2.1
7	CG	118	LEU	2.1
13	AM	19	LEU	2.1
35	DN	51	LEU	2.1
47	DZ	29	LEU	2.1
52	D4	10	LEU	2.1
5	AE	158	GLY	2.1
19	CS	61	PHE	2.1
22	BA	1917	U	2.1
22	DA	1060	U	2.1
37	DP	67	GLY	2.1
39	DR	30	GLY	2.1
9	CI	11	ARG	2.1
10	AJ	37	ARG	2.1
10	CJ	91	ASP	2.1
17	CQ	74	THR	2.1
27	DF	142	ASP	2.1
27	DF	147	ASP	2.1
31	DJ	5	THR	2.1
2	AB	40	ILE	2.1
2	AB	76	ALA	2.1
5	CE	30	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
7	CG	121	ALA	2.1
12	CL	82	ILE	2.1
16	CP	33	ILE	2.1
19	CS	50	ALA	2.1
29	DH	80	ILE	2.1
36	DO	11	ALA	2.1
38	DQ	61	TRP	2.1
2	CB	145	GLU	2.1
2	CB	213	TYR	2.1
53	B5	21	TYR	2.1
26	DE	75	SER	2.0
42	DU	98	SER	2.0
46	DY	1	MET	2.0
1	CA	250	A	2.0
1	CA	1004	A	2.0
9	AI	104	VAL	2.0
9	CI	47	VAL	2.0
22	BA	2114	A	2.0
22	BA	2311	A	2.0
22	DA	781	A	2.0
22	DA	2173	A	2.0
24	DC	17	VAL	2.0
29	BH	9	VAL	2.0
42	DU	34	VAL	2.0
7	CG	2	PRO	2.0
19	AS	9	PRO	2.0
1	AA	83	C	2.0
9	CI	94	LEU	2.0
10	CJ	10	LEU	2.0
22	DA	143	C	2.0
33	DL	95	LEU	2.0
3	AC	37	PHE	2.0
4	CD	73	ARG	2.0
10	AJ	49	PHE	2.0
13	CM	92	ARG	2.0
22	BA	1074	G	2.0
22	BA	2115	G	2.0
22	BA	2307	G	2.0
22	DA	325	G	2.0
24	DC	99	GLY	2.0
30	BI	42	PHE	2.0
36	DO	92	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
43	DV	56	PHE	2.0
43	DV	79	ARG	2.0
47	DZ	15	GLY	2.0
53	B5	191	ARG	2.0
2	AB	20	THR	2.0
9	CI	9	THR	2.0
17	CQ	21	ILE	2.0
22	DA	2180	U	2.0
26	DE	108	ILE	2.0
32	DK	104	THR	2.0
2	AB	209	ALA	2.0
2	CB	12	ALA	2.0
9	AI	16	ALA	2.0
28	DG	60	ASP	2.0
29	BH	36	ALA	2.0
36	DO	6	ALA	2.0
29	DH	76	GLU	2.0
13	CM	23	TYR	2.0
13	CM	62	LYS	2.0
20	AT	64	LYS	2.0
4	AD	36	GLN	2.0
9	AI	48	VAL	2.0
27	DF	118	SER	2.0
1	AA	1019	A	2.0
1	CA	181	A	2.0
1	CA	1280	A	2.0
10	AJ	71	LEU	2.0
10	AJ	87	LEU	2.0
10	CJ	87	LEU	2.0
22	DA	126	A	2.0
22	DA	345	A	2.0
22	DA	1048	A	2.0
22	DA	1067	A	2.0
29	DH	122	LEU	2.0
40	DS	97	LEU	2.0
7	CG	78	ARG	2.0
44	DW	11	ARG	2.0
24	DC	57	GLY	2.0
26	DE	85	PHE	2.0
31	DJ	51	GLY	2.0
53	B5	122	GLY	2.0
1	CA	1214	C	2.0

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Mol	Chain	Res	Type	RSRZ
9	CI	28	ILE	2.0
22	BA	1092	C	2.0
22	DA	183	C	2.0
30	BI	59	ILE	2.0
7	AG	38	THR	2.0
10	CJ	86	ALA	2.0
25	BD	209	ALA	2.0
25	DD	52	THR	2.0
25	DD	129	THR	2.0
36	DO	50	ALA	2.0
46	DY	32	ALA	2.0
53	B5	169	THR	2.0
1	AA	1003	G	2.0
1	CA	973	G	2.0
1	CA	1015	G	2.0
1	CA	1221	G	2.0
1	CA	1312	G	2.0
9	CI	13	LYS	2.0
17	CQ	26	GLU	2.0
22	DA	288	U	2.0
22	DA	2305	U	2.0
27	DF	10	ASP	2.0
22	DA	474	G	2.0
22	DA	805	G	2.0
22	DA	1062	G	2.0
22	DA	1210	G	2.0
22	DA	2294	G	2.0
22	DA	2383	G	2.0
41	DT	4	GLU	2.0
5	AE	152	MET	2.0
36	DO	99	TYR	2.0
12	CL	33	VAL	2.0
36	DO	39	VAL	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 ⓘ

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(Å ²)	Q<0.9
54	MG	DA	3077	1/1	0.02	0.19	115,115,115,115	0
54	MG	DA	3119	1/1	0.33	0.30	112,112,112,112	0
54	MG	DA	3135	1/1	0.33	0.31	101,101,101,101	0
54	MG	DA	3133	1/1	0.46	0.46	105,105,105,105	0
54	MG	DA	3041	1/1	0.52	0.39	72,72,72,72	0
54	MG	DA	3028	1/1	0.55	0.34	104,104,104,104	0
54	MG	DA	3048	1/1	0.55	0.10	123,123,123,123	0
54	MG	BA	3194	1/1	0.56	0.28	41,41,41,41	0
54	MG	AA	1656	1/1	0.59	0.26	66,66,66,66	0
54	MG	DA	3061	1/1	0.59	1.04	102,102,102,102	0
54	MG	DL	201	1/1	0.59	0.30	68,68,68,68	0
54	MG	BA	3137	1/1	0.60	0.38	46,46,46,46	0
54	MG	DA	3092	1/1	0.61	0.28	117,117,117,117	0
54	MG	DA	3003	1/1	0.62	0.29	101,101,101,101	0
54	MG	DA	3099	1/1	0.62	0.28	91,91,91,91	0
54	MG	DA	3137	1/1	0.63	0.29	52,52,52,52	0
54	MG	CA	1636	1/1	0.66	0.15	127,127,127,127	0
54	MG	DA	3026	1/1	0.66	0.25	100,100,100,100	0
54	MG	AA	1662	1/1	0.68	0.27	58,58,58,58	0
54	MG	DA	3062	1/1	0.68	0.34	89,89,89,89	0
54	MG	DA	3005	1/1	0.69	0.21	103,103,103,103	0
54	MG	DA	3126	1/1	0.69	0.13	77,77,77,77	0
54	MG	AA	1650	1/1	0.70	0.37	61,61,61,61	0
54	MG	DA	3100	1/1	0.70	0.18	86,86,86,86	0
54	MG	DA	3007	1/1	0.71	0.12	119,119,119,119	0
54	MG	DA	3143	1/1	0.72	0.12	73,73,73,73	0
54	MG	DA	3035	1/1	0.72	0.12	79,79,79,79	0
54	MG	DA	3115	1/1	0.73	0.12	113,113,113,113	0
54	MG	AA	1658	1/1	0.74	0.20	52,52,52,52	0
54	MG	CA	1655	1/1	0.74	0.19	45,45,45,45	0
54	MG	AA	1666	1/1	0.74	0.10	61,61,61,61	0
54	MG	DA	3145	1/1	0.74	0.15	56,56,56,56	0
54	MG	CA	1635	1/1	0.74	0.13	122,122,122,122	0
54	MG	DA	3058	1/1	0.75	0.45	107,107,107,107	0
54	MG	AA	1669	1/1	0.76	0.26	45,45,45,45	0
54	MG	DA	3019	1/1	0.76	0.14	109,109,109,109	0
54	MG	DA	3025	1/1	0.76	0.16	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	CA	1653	1/1	0.77	0.20	47,47,47,47	0
54	MG	DA	3029	1/1	0.77	0.19	77,77,77,77	0
54	MG	DA	3162	1/1	0.77	0.15	63,63,63,63	0
54	MG	DA	3140	1/1	0.77	0.20	42,42,42,42	0
54	MG	DA	3157	1/1	0.78	0.11	76,76,76,76	0
54	MG	BA	3078	1/1	0.78	0.28	87,87,87,87	0
54	MG	AA	1664	1/1	0.78	0.14	49,49,49,49	0
54	MG	DA	3071	1/1	0.79	0.15	87,87,87,87	0
54	MG	BA	3075	1/1	0.79	0.14	35,35,35,35	0
54	MG	DA	3078	1/1	0.79	0.12	110,110,110,110	0
54	MG	DA	3149	1/1	0.80	0.13	55,55,55,55	0
54	MG	DA	3044	1/1	0.80	0.14	113,113,113,113	0
54	MG	AA	1647	1/1	0.80	0.18	48,48,48,48	0
54	MG	DA	3163	1/1	0.80	0.18	64,64,64,64	0
54	MG	DA	3131	1/1	0.80	0.28	94,94,94,94	0
54	MG	DA	3113	1/1	0.81	0.13	72,72,72,72	0
54	MG	AA	1651	1/1	0.81	0.23	51,51,51,51	0
54	MG	CA	1646	1/1	0.81	0.14	97,97,97,97	0
54	MG	DA	3027	1/1	0.81	0.10	97,97,97,97	0
54	MG	BA	3063	1/1	0.81	0.38	52,52,52,52	0
54	MG	DA	3093	1/1	0.81	0.17	94,94,94,94	0
54	MG	DA	3014	1/1	0.81	0.15	78,78,78,78	0
54	MG	BA	3134	1/1	0.81	0.36	54,54,54,54	0
54	MG	BA	3125	1/1	0.82	0.25	39,39,39,39	0
54	MG	DA	3072	1/1	0.82	0.24	86,86,86,86	0
54	MG	CA	1652	1/1	0.82	0.10	86,86,86,86	0
54	MG	BA	3027	1/1	0.82	0.25	44,44,44,44	0
54	MG	AA	1643	1/1	0.82	0.11	42,42,42,42	0
54	MG	DA	3042	1/1	0.82	0.10	87,87,87,87	0
54	MG	AA	1661	1/1	0.83	0.20	55,55,55,55	0
54	MG	CA	1631	1/1	0.83	0.10	101,101,101,101	0
54	MG	DA	3017	1/1	0.83	0.18	100,100,100,100	0
54	MG	DA	3070	1/1	0.83	0.06	108,108,108,108	0
54	MG	DA	3142	1/1	0.83	0.14	34,34,34,34	0
54	MG	CA	1632	1/1	0.83	0.11	79,79,79,79	0
54	MG	AA	1642	1/1	0.83	0.08	32,32,32,32	0
54	MG	DA	3116	1/1	0.83	0.17	72,72,72,72	0
54	MG	BA	3049	1/1	0.83	0.13	50,50,50,50	0
54	MG	DA	3158	1/1	0.83	0.12	52,52,52,52	0
54	MG	DA	3120	1/1	0.83	0.16	81,81,81,81	0
54	MG	CA	1645	1/1	0.83	0.13	28,28,28,28	0
54	MG	DA	3091	1/1	0.83	0.10	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3075	1/1	0.84	0.12	83,83,83,83	0
54	MG	DA	3060	1/1	0.84	0.16	81,81,81,81	0
54	MG	CA	1642	1/1	0.84	0.19	25,25,25,25	0
54	MG	BA	3120	1/1	0.84	0.15	47,47,47,47	0
54	MG	CA	1656	1/1	0.84	0.06	50,50,50,50	0
54	MG	CA	1630	1/1	0.84	0.14	120,120,120,120	0
54	MG	AA	1653	1/1	0.84	0.21	47,47,47,47	0
54	MG	CA	1643	1/1	0.85	0.24	44,44,44,44	0
54	MG	BA	3178	1/1	0.85	0.21	27,27,27,27	0
54	MG	AA	1659	1/1	0.85	0.11	62,62,62,62	0
54	MG	DA	3151	1/1	0.85	0.35	56,56,56,56	0
54	MG	DA	3106	1/1	0.85	0.11	49,49,49,49	0
54	MG	CA	1633	1/1	0.85	0.41	76,76,76,76	0
54	MG	BA	3195	1/1	0.85	0.28	31,31,31,31	0
54	MG	CA	1604	1/1	0.85	0.10	95,95,95,95	0
54	MG	DA	3165	1/1	0.85	0.10	100,100,100,100	0
54	MG	AA	1668	1/1	0.85	0.17	54,54,54,54	0
55	DOL	DA	3001	48/48	0.85	0.18	28,49,62,81	0
54	MG	BA	3085	1/1	0.86	0.16	29,29,29,29	0
54	MG	DA	3147	1/1	0.86	0.30	67,67,67,67	0
54	MG	AA	1654	1/1	0.86	0.12	34,34,34,34	0
54	MG	DA	3150	1/1	0.86	0.28	50,50,50,50	0
54	MG	DA	3111	1/1	0.86	0.12	103,103,103,103	0
54	MG	DA	3011	1/1	0.86	0.09	73,73,73,73	0
54	MG	DA	3112	1/1	0.87	0.32	92,92,92,92	0
54	MG	CA	1649	1/1	0.87	0.18	61,61,61,61	0
54	MG	AA	1631	1/1	0.87	0.09	52,52,52,52	0
54	MG	AA	1634	1/1	0.87	0.22	73,73,73,73	0
54	MG	DA	3161	1/1	0.87	0.16	46,46,46,46	0
54	MG	AA	1657	1/1	0.87	0.10	60,60,60,60	0
54	MG	BA	3173	1/1	0.87	0.12	38,38,38,38	0
54	MG	DA	3032	1/1	0.87	0.14	71,71,71,71	0
54	MG	DA	3127	1/1	0.87	0.11	74,74,74,74	0
54	MG	CA	1628	1/1	0.87	0.18	99,99,99,99	0
54	MG	BA	3172	1/1	0.88	0.13	27,27,27,27	0
54	MG	DA	3123	1/1	0.88	0.09	62,62,62,62	0
54	MG	DA	3136	1/1	0.88	0.11	94,94,94,94	0
54	MG	DA	3056	1/1	0.88	0.23	91,91,91,91	0
54	MG	BA	3016	1/1	0.88	0.27	51,51,51,51	0
54	MG	CA	1615	1/1	0.88	0.19	52,52,52,52	0
54	MG	DA	3152	1/1	0.88	0.17	45,45,45,45	0
54	MG	DA	3156	1/1	0.88	0.13	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	AA	1629	1/1	0.89	0.20	79,79,79,79	0
54	MG	DA	3037	1/1	0.89	0.09	92,92,92,92	0
54	MG	BA	3136	1/1	0.89	0.16	24,24,24,24	0
54	MG	BA	3189	1/1	0.89	0.13	48,48,48,48	0
54	MG	AA	1618	1/1	0.89	0.20	75,75,75,75	0
54	MG	BA	3168	1/1	0.89	0.20	41,41,41,41	0
54	MG	DA	3049	1/1	0.89	0.10	87,87,87,87	0
54	MG	CA	1602	1/1	0.89	0.10	87,87,87,87	0
54	MG	DA	3009	1/1	0.89	0.12	91,91,91,91	0
54	MG	DA	3144	1/1	0.89	0.10	72,72,72,72	0
54	MG	AA	1670	1/1	0.89	0.21	58,58,58,58	0
54	MG	DA	3012	1/1	0.89	0.14	78,78,78,78	0
54	MG	DA	3148	1/1	0.89	0.24	41,41,41,41	0
54	MG	BA	3062	1/1	0.90	0.26	46,46,46,46	0
54	MG	AA	1663	1/1	0.90	0.08	45,45,45,45	0
54	MG	DA	3154	1/1	0.90	0.12	57,57,57,57	0
54	MG	DA	3141	1/1	0.90	0.21	39,39,39,39	0
54	MG	AA	1645	1/1	0.90	0.12	54,54,54,54	0
54	MG	DA	3124	1/1	0.90	0.07	87,87,87,87	0
54	MG	CA	1614	1/1	0.90	0.09	49,49,49,49	0
54	MG	AM	201	1/1	0.90	0.15	59,59,59,59	0
54	MG	DA	3057	1/1	0.90	0.08	92,92,92,92	0
54	MG	BA	3059	1/1	0.90	0.26	36,36,36,36	0
54	MG	CA	1629	1/1	0.90	0.08	89,89,89,89	0
54	MG	BA	3146	1/1	0.90	0.22	32,32,32,32	0
54	MG	BA	3090	1/1	0.91	0.17	34,34,34,34	0
54	MG	BA	3042	1/1	0.91	0.19	2,2,2,2	0
54	MG	CA	1651	1/1	0.91	0.08	42,42,42,42	0
54	MG	DA	3098	1/1	0.91	0.10	60,60,60,60	0
54	MG	DA	3068	1/1	0.91	0.10	64,64,64,64	0
54	MG	BA	3082	1/1	0.91	0.09	16,16,16,16	0
54	MG	BA	3183	1/1	0.91	0.08	19,19,19,19	0
54	MG	CA	1654	1/1	0.91	0.08	55,55,55,55	0
54	MG	CA	1608	1/1	0.91	0.10	80,80,80,80	0
54	MG	DA	3159	1/1	0.91	0.09	47,47,47,47	0
54	MG	DA	3034	1/1	0.91	0.11	69,69,69,69	0
54	MG	AA	1637	1/1	0.91	0.09	81,81,81,81	0
54	MG	DA	3079	1/1	0.91	0.08	98,98,98,98	0
54	MG	DA	3080	1/1	0.91	0.10	96,96,96,96	0
54	MG	DA	3084	1/1	0.91	0.07	104,104,104,104	0
54	MG	DA	3088	1/1	0.91	0.08	75,75,75,75	0
54	MG	DA	3040	1/1	0.92	0.06	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3031	1/1	0.92	0.10	20,20,20,20	0
54	MG	BA	3005	1/1	0.92	0.11	45,45,45,45	0
54	MG	DA	3016	1/1	0.92	0.19	73,73,73,73	0
54	MG	BA	3089	1/1	0.92	0.10	24,24,24,24	0
54	MG	AA	1622	1/1	0.92	0.09	50,50,50,50	0
54	MG	BA	3190	1/1	0.92	0.13	39,39,39,39	0
54	MG	BA	3100	1/1	0.92	0.25	51,51,51,51	0
54	MG	DA	3089	1/1	0.92	0.09	87,87,87,87	0
54	MG	BA	3149	1/1	0.92	0.14	44,44,44,44	0
54	MG	BA	3155	1/1	0.92	0.09	18,18,18,18	0
54	MG	BA	3162	1/1	0.92	0.06	21,21,21,21	0
54	MG	DA	3094	1/1	0.92	0.12	87,87,87,87	0
54	MG	DA	3095	1/1	0.92	0.10	91,91,91,91	0
54	MG	CA	1637	1/1	0.92	0.12	64,64,64,64	0
54	MG	CA	1606	1/1	0.92	0.10	90,90,90,90	0
54	MG	DA	3138	1/1	0.92	0.20	38,38,38,38	0
54	MG	AA	1667	1/1	0.92	0.09	30,30,30,30	0
54	MG	DA	3103	1/1	0.92	0.09	67,67,67,67	0
54	MG	BA	3124	1/1	0.92	0.09	20,20,20,20	0
54	MG	DA	3046	1/1	0.93	0.09	68,68,68,68	0
54	MG	BA	3165	1/1	0.93	0.24	38,38,38,38	0
54	MG	DA	3024	1/1	0.93	0.10	46,46,46,46	0
54	MG	BA	3113	1/1	0.93	0.13	39,39,39,39	0
54	MG	BA	3086	1/1	0.93	0.11	24,24,24,24	0
54	MG	DA	3090	1/1	0.93	0.07	84,84,84,84	0
54	MG	BA	3036	1/1	0.93	0.17	10,10,10,10	0
54	MG	DA	3125	1/1	0.93	0.10	59,59,59,59	0
54	MG	BA	3147	1/1	0.93	0.16	23,23,23,23	0
54	MG	BA	3057	1/1	0.93	0.17	68,68,68,68	0
54	MG	CA	1621	1/1	0.93	0.10	72,72,72,72	0
54	MG	DA	3132	1/1	0.93	0.18	64,64,64,64	0
54	MG	DA	3008	1/1	0.93	0.12	102,102,102,102	0
54	MG	CA	1627	1/1	0.93	0.16	87,87,87,87	0
54	MG	BA	3150	1/1	0.93	0.17	29,29,29,29	0
54	MG	BA	3151	1/1	0.93	0.16	12,12,12,12	0
54	MG	DA	3073	1/1	0.93	0.14	61,61,61,61	0
54	MG	DA	3164	1/1	0.93	0.24	40,40,40,40	0
54	MG	CA	1650	1/1	0.93	0.09	42,42,42,42	0
54	MG	DB	203	1/1	0.93	0.08	85,85,85,85	0
54	MG	BA	3132	1/1	0.93	0.21	27,27,27,27	0
54	MG	D2	101	1/1	0.93	0.09	76,76,76,76	0
54	MG	AA	1628	1/1	0.93	0.08	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	CA	1612	1/1	0.94	0.09	46,46,46,46	0
54	MG	DA	3047	1/1	0.94	0.08	74,74,74,74	0
54	MG	AA	1633	1/1	0.94	0.07	51,51,51,51	0
54	MG	BA	3187	1/1	0.94	0.18	30,30,30,30	0
54	MG	DA	3087	1/1	0.94	0.07	64,64,64,64	0
54	MG	CA	1617	1/1	0.94	0.11	57,57,57,57	0
54	MG	AA	1649	1/1	0.94	0.10	32,32,32,32	0
54	MG	BA	3169	1/1	0.94	0.07	29,29,29,29	0
54	MG	DA	3033	1/1	0.94	0.07	63,63,63,63	0
54	MG	DA	3153	1/1	0.94	0.16	45,45,45,45	0
54	MG	BA	3170	1/1	0.94	0.09	36,36,36,36	0
54	MG	DA	3155	1/1	0.94	0.17	42,42,42,42	0
54	MG	BA	3061	1/1	0.94	0.23	40,40,40,40	0
54	MG	BA	3159	1/1	0.94	0.13	8,8,8,8	0
54	MG	DA	3128	1/1	0.94	0.06	79,79,79,79	0
54	MG	DA	3039	1/1	0.94	0.05	57,57,57,57	0
54	MG	DA	3097	1/1	0.94	0.10	87,87,87,87	0
54	MG	BA	3174	1/1	0.94	0.06	14,14,14,14	0
54	MG	CA	1605	1/1	0.94	0.09	86,86,86,86	0
54	MG	BA	3176	1/1	0.94	0.13	28,28,28,28	0
54	MG	DA	3101	1/1	0.94	0.06	63,63,63,63	0
54	MG	DB	201	1/1	0.94	0.07	113,113,113,113	0
54	MG	DA	3102	1/1	0.94	0.06	61,61,61,61	0
54	MG	AA	1624	1/1	0.94	0.09	46,46,46,46	0
54	MG	DA	3104	1/1	0.94	0.06	80,80,80,80	0
54	MG	DA	3045	1/1	0.94	0.10	87,87,87,87	0
54	MG	DA	3006	1/1	0.95	0.05	95,95,95,95	0
54	MG	DA	3134	1/1	0.95	0.07	54,54,54,54	0
54	MG	AA	1639	1/1	0.95	0.12	45,45,45,45	0
54	MG	BA	3185	1/1	0.95	0.15	13,13,13,13	0
54	MG	BA	3115	1/1	0.95	0.06	17,17,17,17	0
54	MG	DA	3010	1/1	0.95	0.04	80,80,80,80	0
54	MG	DA	3139	1/1	0.95	0.16	31,31,31,31	0
54	MG	DA	3096	1/1	0.95	0.07	61,61,61,61	0
54	MG	BA	3116	1/1	0.95	0.17	32,32,32,32	0
54	MG	BA	3154	1/1	0.95	0.06	12,12,12,12	0
54	MG	BA	3192	1/1	0.95	0.09	23,23,23,23	0
54	MG	AA	1648	1/1	0.95	0.07	33,33,33,33	0
54	MG	BA	3076	1/1	0.95	0.15	33,33,33,33	0
54	MG	BQ	201	1/1	0.95	0.11	7,7,7,7	0
54	MG	DA	3023	1/1	0.95	0.06	76,76,76,76	0
54	MG	AA	1655	1/1	0.95	0.11	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3105	1/1	0.95	0.12	81,81,81,81	0
54	MG	DA	3069	1/1	0.95	0.11	80,80,80,80	0
54	MG	DA	3109	1/1	0.95	0.10	47,47,47,47	0
54	MG	DA	3110	1/1	0.95	0.11	39,39,39,39	0
54	MG	CA	1644	1/1	0.95	0.14	43,43,43,43	0
54	MG	AA	1612	1/1	0.95	0.07	48,48,48,48	0
54	MG	BA	3167	1/1	0.95	0.10	32,32,32,32	0
54	MG	CA	1648	1/1	0.95	0.12	19,19,19,19	0
54	MG	BA	3133	1/1	0.95	0.20	39,39,39,39	0
54	MG	DA	3117	1/1	0.95	0.06	72,72,72,72	0
54	MG	DA	3160	1/1	0.95	0.06	64,64,64,64	0
54	MG	AA	1602	1/1	0.95	0.24	55,55,55,55	0
54	MG	CA	1610	1/1	0.95	0.06	65,65,65,65	0
54	MG	AA	1665	1/1	0.95	0.10	47,47,47,47	0
54	MG	BA	3171	1/1	0.95	0.12	28,28,28,28	0
54	MG	DA	3083	1/1	0.95	0.13	74,74,74,74	0
54	MG	BA	3012	1/1	0.95	0.09	19,19,19,19	0
54	MG	BA	3140	1/1	0.95	0.18	0,0,0,0	0
54	MG	AA	1638	1/1	0.95	0.06	64,64,64,64	0
54	MG	BA	3017	1/1	0.95	0.11	13,13,13,13	0
54	MG	BA	3148	1/1	0.95	0.17	28,28,28,28	0
54	MG	CA	1603	1/1	0.96	0.06	37,37,37,37	0
54	MG	BA	3179	1/1	0.96	0.12	30,30,30,30	0
54	MG	AA	1660	1/1	0.96	0.06	45,45,45,45	0
54	MG	BA	3184	1/1	0.96	0.09	3,3,3,3	0
54	MG	AA	1614	1/1	0.96	0.15	74,74,74,74	0
54	MG	BA	3093	1/1	0.96	0.06	57,57,57,57	0
54	MG	CA	1611	1/1	0.96	0.12	87,87,87,87	0
54	MG	DA	3130	1/1	0.96	0.06	80,80,80,80	0
54	MG	BA	3157	1/1	0.96	0.07	18,18,18,18	0
54	MG	DA	3081	1/1	0.96	0.08	66,66,66,66	0
54	MG	BA	3158	1/1	0.96	0.15	22,22,22,22	0
54	MG	AA	1610	1/1	0.96	0.12	65,65,65,65	0
54	MG	DA	3108	1/1	0.96	0.09	61,61,61,61	0
54	MG	AA	1619	1/1	0.96	0.05	71,71,71,71	0
54	MG	BA	3175	1/1	0.96	0.06	34,34,34,34	0
54	MG	CA	1647	1/1	0.96	0.09	36,36,36,36	0
54	MG	BA	3038	1/1	0.96	0.15	31,31,31,31	0
54	MG	DA	3066	1/1	0.96	0.07	58,58,58,58	0
54	MG	DA	3114	1/1	0.96	0.05	66,66,66,66	0
54	MG	DA	3067	1/1	0.96	0.06	53,53,53,53	0
54	MG	CA	1601	1/1	0.96	0.07	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	AA	1608	1/1	0.96	0.07	27,27,27,27	0
54	MG	DQ	201	1/1	0.96	0.17	37,37,37,37	0
54	MG	DA	3015	1/1	0.96	0.08	63,63,63,63	0
55	DOL	BA	3001	48/48	0.96	0.09	1,7,30,58	0
54	MG	DA	3146	1/1	0.96	0.29	48,48,48,48	0
54	MG	BA	3161	1/1	0.97	0.12	33,33,33,33	0
54	MG	BB	204	1/1	0.97	0.23	12,12,12,12	0
54	MG	DA	3021	1/1	0.97	0.07	53,53,53,53	0
54	MG	DA	3022	1/1	0.97	0.05	55,55,55,55	0
54	MG	DA	3074	1/1	0.97	0.08	72,72,72,72	0
54	MG	CA	1638	1/1	0.97	0.06	65,65,65,65	0
54	MG	CA	1639	1/1	0.97	0.05	49,49,49,49	0
54	MG	CA	1640	1/1	0.97	0.07	27,27,27,27	0
54	MG	CA	1641	1/1	0.97	0.16	66,66,66,66	0
54	MG	BA	3058	1/1	0.97	0.12	9,9,9,9	0
54	MG	BA	3003	1/1	0.97	0.08	18,18,18,18	0
54	MG	AA	1626	1/1	0.97	0.14	53,53,53,53	0
54	MG	DA	3031	1/1	0.97	0.06	65,65,65,65	0
54	MG	DA	3085	1/1	0.97	0.10	76,76,76,76	0
54	MG	DA	3086	1/1	0.97	0.06	74,74,74,74	0
54	MG	AA	1609	1/1	0.97	0.10	35,35,35,35	0
54	MG	AA	1644	1/1	0.97	0.10	45,45,45,45	0
54	MG	BA	3138	1/1	0.97	0.22	1,1,1,1	0
54	MG	BA	3094	1/1	0.97	0.10	42,42,42,42	0
54	MG	CA	1607	1/1	0.97	0.05	53,53,53,53	0
54	MG	DA	3038	1/1	0.97	0.05	64,64,64,64	0
54	MG	BA	3142	1/1	0.97	0.24	0,0,0,0	0
54	MG	BA	3095	1/1	0.97	0.04	17,17,17,17	0
54	MG	BA	3069	1/1	0.97	0.07	1,1,1,1	0
54	MG	BA	3112	1/1	0.97	0.05	29,29,29,29	0
54	MG	DA	3043	1/1	0.97	0.08	68,68,68,68	0
54	MG	BA	3073	1/1	0.97	0.14	12,12,12,12	0
54	MG	BA	3048	1/1	0.97	0.07	9,9,9,9	0
54	MG	AA	1605	1/1	0.97	0.08	26,26,26,26	0
54	MG	DA	3002	1/1	0.97	0.07	78,78,78,78	0
54	MG	CA	1619	1/1	0.97	0.05	34,34,34,34	0
54	MG	BA	3180	1/1	0.97	0.06	29,29,29,29	0
54	MG	DA	3052	1/1	0.97	0.06	60,60,60,60	0
54	MG	DA	3053	1/1	0.97	0.05	44,44,44,44	0
54	MG	DA	3055	1/1	0.97	0.06	59,59,59,59	0
54	MG	CA	1622	1/1	0.97	0.06	46,46,46,46	0
54	MG	CA	1626	1/1	0.97	0.12	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3153	1/1	0.97	0.07	26,26,26,26	0
54	MG	BA	3119	1/1	0.97	0.04	21,21,21,21	0
54	MG	BA	3050	1/1	0.97	0.08	18,18,18,18	0
54	MG	BA	3156	1/1	0.97	0.19	26,26,26,26	0
54	MG	DA	3063	1/1	0.97	0.06	50,50,50,50	0
54	MG	DA	3064	1/1	0.97	0.06	53,53,53,53	0
54	MG	DA	3065	1/1	0.97	0.05	34,34,34,34	0
54	MG	BA	3122	1/1	0.97	0.07	25,25,25,25	0
54	MG	BA	3081	1/1	0.97	0.05	18,18,18,18	0
54	MG	BA	3002	1/1	0.97	0.04	19,19,19,19	0
54	MG	BA	3160	1/1	0.97	0.03	3,3,3,3	0
54	MG	DA	3018	1/1	0.98	0.05	55,55,55,55	0
54	MG	DA	3121	1/1	0.98	0.05	48,48,48,48	0
54	MG	DA	3122	1/1	0.98	0.05	36,36,36,36	0
54	MG	BA	3054	1/1	0.98	0.07	6,6,6,6	0
54	MG	DA	3020	1/1	0.98	0.10	49,49,49,49	0
54	MG	BA	3182	1/1	0.98	0.10	16,16,16,16	0
54	MG	BA	3004	1/1	0.98	0.04	22,22,22,22	0
54	MG	AA	1615	1/1	0.98	0.05	62,62,62,62	0
54	MG	BA	3096	1/1	0.98	0.04	19,19,19,19	0
54	MG	DA	3129	1/1	0.98	0.07	50,50,50,50	0
54	MG	CA	1634	1/1	0.98	0.04	51,51,51,51	0
54	MG	BA	3186	1/1	0.98	0.16	14,14,14,14	0
54	MG	BA	3097	1/1	0.98	0.05	8,8,8,8	0
54	MG	BA	3008	1/1	0.98	0.10	33,33,33,33	0
54	MG	BA	3152	1/1	0.98	0.10	12,12,12,12	0
54	MG	DA	3082	1/1	0.98	0.05	59,59,59,59	0
54	MG	BA	3191	1/1	0.98	0.19	12,12,12,12	0
54	MG	BA	3104	1/1	0.98	0.10	8,8,8,8	0
54	MG	BA	3193	1/1	0.98	0.04	32,32,32,32	0
54	MG	BA	3105	1/1	0.98	0.04	10,10,10,10	0
54	MG	AA	1627	1/1	0.98	0.05	48,48,48,48	0
54	MG	DA	3036	1/1	0.98	0.05	62,62,62,62	0
54	MG	BB	202	1/1	0.98	0.04	6,6,6,6	0
54	MG	AA	1616	1/1	0.98	0.05	57,57,57,57	0
54	MG	AA	1607	1/1	0.98	0.06	54,54,54,54	0
54	MG	BA	3064	1/1	0.98	0.04	1,1,1,1	0
54	MG	BA	3021	1/1	0.98	0.11	0,0,0,0	0
54	MG	BA	3071	1/1	0.98	0.10	66,66,66,66	0
54	MG	AA	1630	1/1	0.98	0.05	35,35,35,35	0
54	MG	AA	1601	1/1	0.98	0.05	53,53,53,53	0
54	MG	BA	3163	1/1	0.98	0.24	12,12,12,12	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3033	1/1	0.98	0.04	9,9,9,9	0
54	MG	BA	3166	1/1	0.98	0.09	23,23,23,23	0
54	MG	CA	1609	1/1	0.98	0.04	87,87,87,87	0
54	MG	BA	3077	1/1	0.98	0.05	12,12,12,12	0
54	MG	AA	1646	1/1	0.98	0.04	54,54,54,54	0
54	MG	AA	1613	1/1	0.98	0.09	33,33,33,33	0
54	MG	DA	3054	1/1	0.98	0.06	48,48,48,48	0
54	MG	DA	3004	1/1	0.98	0.06	78,78,78,78	0
54	MG	CA	1613	1/1	0.98	0.04	20,20,20,20	0
54	MG	DA	3107	1/1	0.98	0.06	70,70,70,70	0
54	MG	BA	3135	1/1	0.98	0.05	3,3,3,3	0
54	MG	AA	1623	1/1	0.98	0.07	41,41,41,41	0
54	MG	CA	1616	1/1	0.98	0.05	38,38,38,38	0
54	MG	AN	201	1/1	0.98	0.12	62,62,62,62	0
54	MG	AA	1635	1/1	0.98	0.08	23,23,23,23	0
54	MG	AA	1606	1/1	0.98	0.04	44,44,44,44	0
54	MG	DB	202	1/1	0.98	0.09	64,64,64,64	0
54	MG	BA	3141	1/1	0.98	0.07	17,17,17,17	0
54	MG	CA	1623	1/1	0.98	0.11	50,50,50,50	0
54	MG	BA	3052	1/1	0.98	0.04	7,7,7,7	0
54	MG	BA	3143	1/1	0.98	0.24	22,22,22,22	0
54	MG	DA	3118	1/1	0.98	0.04	55,55,55,55	0
54	MG	BA	3145	1/1	0.98	0.13	17,17,17,17	0
54	MG	BA	3045	1/1	0.99	0.03	27,27,27,27	0
54	MG	BA	3046	1/1	0.99	0.07	6,6,6,6	0
54	MG	BA	3047	1/1	0.99	0.05	4,4,4,4	0
54	MG	BA	3164	1/1	0.99	0.03	4,4,4,4	0
54	MG	AA	1652	1/1	0.99	0.07	18,18,18,18	0
54	MG	BA	3006	1/1	0.99	0.07	43,43,43,43	0
54	MG	BA	3103	1/1	0.99	0.05	0,0,0,0	0
54	MG	BA	3007	1/1	0.99	0.04	24,24,24,24	0
54	MG	BA	3051	1/1	0.99	0.04	1,1,1,1	0
54	MG	BA	3106	1/1	0.99	0.08	5,5,5,5	0
54	MG	BA	3107	1/1	0.99	0.07	0,0,0,0	0
54	MG	BA	3111	1/1	0.99	0.07	4,4,4,4	0
54	MG	AA	1641	1/1	0.99	0.03	24,24,24,24	0
54	MG	BA	3053	1/1	0.99	0.04	6,6,6,6	0
54	MG	DA	3050	1/1	0.99	0.03	48,48,48,48	0
54	MG	DA	3051	1/1	0.99	0.04	32,32,32,32	0
54	MG	BA	3009	1/1	0.99	0.04	4,4,4,4	0
54	MG	BA	3056	1/1	0.99	0.04	2,2,2,2	0
54	MG	BA	3177	1/1	0.99	0.11	12,12,12,12	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3117	1/1	0.99	0.06	2,2,2,2	0
54	MG	BA	3118	1/1	0.99	0.03	4,4,4,4	0
54	MG	BA	3011	1/1	0.99	0.04	0,0,0,0	0
54	MG	BA	3181	1/1	0.99	0.11	16,16,16,16	0
54	MG	DA	3059	1/1	0.99	0.05	39,39,39,39	0
54	MG	AA	1611	1/1	0.99	0.03	20,20,20,20	0
54	MG	BA	3121	1/1	0.99	0.03	2,2,2,2	0
54	MG	BA	3015	1/1	0.99	0.06	4,4,4,4	0
54	MG	BA	3060	1/1	0.99	0.04	14,14,14,14	0
54	MG	AA	1632	1/1	0.99	0.03	37,37,37,37	0
54	MG	BA	3127	1/1	0.99	0.06	5,5,5,5	0
54	MG	BA	3188	1/1	0.99	0.04	6,6,6,6	0
54	MG	BA	3129	1/1	0.99	0.05	3,3,3,3	0
54	MG	BA	3130	1/1	0.99	0.05	0,0,0,0	0
54	MG	AA	1625	1/1	0.99	0.08	14,14,14,14	0
54	MG	BA	3020	1/1	0.99	0.04	24,24,24,24	0
54	MG	AA	1603	1/1	0.99	0.10	44,44,44,44	0
54	MG	BA	3065	1/1	0.99	0.06	1,1,1,1	0
54	MG	BA	3022	1/1	0.99	0.04	16,16,16,16	0
54	MG	BB	201	1/1	0.99	0.03	31,31,31,31	0
54	MG	BA	3025	1/1	0.99	0.04	2,2,2,2	0
54	MG	DA	3076	1/1	0.99	0.05	66,66,66,66	0
54	MG	BA	3072	1/1	0.99	0.03	7,7,7,7	0
54	MG	BA	3139	1/1	0.99	0.20	0,0,0,0	0
54	MG	BA	3026	1/1	0.99	0.03	3,3,3,3	0
54	MG	AA	1620	1/1	0.99	0.03	30,30,30,30	0
54	MG	BA	3029	1/1	0.99	0.15	23,23,23,23	0
54	MG	DA	3013	1/1	0.99	0.05	45,45,45,45	0
54	MG	BA	3030	1/1	0.99	0.04	6,6,6,6	0
54	MG	BA	3144	1/1	0.99	0.13	6,6,6,6	0
54	MG	AA	1636	1/1	0.99	0.03	17,17,17,17	0
54	MG	BA	3079	1/1	0.99	0.03	22,22,22,22	0
54	MG	BA	3080	1/1	0.99	0.03	42,42,42,42	0
54	MG	BA	3032	1/1	0.99	0.07	5,5,5,5	0
54	MG	AA	1621	1/1	0.99	0.09	19,19,19,19	0
54	MG	BA	3083	1/1	0.99	0.05	2,2,2,2	0
54	MG	BA	3084	1/1	0.99	0.11	16,16,16,16	0
54	MG	BA	3034	1/1	0.99	0.04	2,2,2,2	0
54	MG	BA	3035	1/1	0.99	0.04	3,3,3,3	0
54	MG	BA	3087	1/1	0.99	0.04	2,2,2,2	0
54	MG	BA	3088	1/1	0.99	0.10	2,2,2,2	0
54	MG	AA	1604	1/1	0.99	0.03	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	CA	1618	1/1	0.99	0.06	35,35,35,35	0
54	MG	AA	1617	1/1	0.99	0.03	42,42,42,42	0
54	MG	DA	3030	1/1	0.99	0.09	70,70,70,70	0
54	MG	CA	1620	1/1	0.99	0.04	61,61,61,61	0
54	MG	BA	3091	1/1	0.99	0.03	4,4,4,4	0
54	MG	BA	3092	1/1	0.99	0.02	21,21,21,21	0
54	MG	AA	1640	1/1	0.99	0.04	21,21,21,21	0
54	MG	CA	1624	1/1	0.99	0.03	39,39,39,39	0
56	ZN	D4	101	1/1	0.99	0.02	91,91,91,91	0
54	MG	BA	3128	1/1	1.00	0.03	0,0,0,0	0
54	MG	BA	3098	1/1	1.00	0.02	3,3,3,3	0
54	MG	BA	3099	1/1	1.00	0.07	5,5,5,5	0
54	MG	BA	3131	1/1	1.00	0.05	1,1,1,1	0
54	MG	BA	3043	1/1	1.00	0.05	5,5,5,5	0
54	MG	BA	3101	1/1	1.00	0.03	1,1,1,1	0
54	MG	BB	203	1/1	1.00	0.05	8,8,8,8	0
54	MG	BA	3102	1/1	1.00	0.02	9,9,9,9	0
54	MG	BA	3044	1/1	1.00	0.04	3,3,3,3	0
54	MG	BA	3023	1/1	1.00	0.02	1,1,1,1	0
54	MG	BA	3024	1/1	1.00	0.05	0,0,0,0	0
54	MG	BA	3018	1/1	1.00	0.05	0,0,0,0	0
54	MG	BA	3019	1/1	1.00	0.02	14,14,14,14	0
54	MG	BA	3108	1/1	1.00	0.09	1,1,1,1	0
54	MG	BA	3109	1/1	1.00	0.04	6,6,6,6	0
54	MG	BA	3110	1/1	1.00	0.10	4,4,4,4	0
54	MG	BA	3010	1/1	1.00	0.03	0,0,0,0	0
54	MG	BA	3028	1/1	1.00	0.05	6,6,6,6	0
54	MG	BA	3066	1/1	1.00	0.04	0,0,0,0	0
54	MG	BA	3114	1/1	1.00	0.05	0,0,0,0	0
54	MG	BA	3067	1/1	1.00	0.07	1,1,1,1	0
54	MG	BA	3068	1/1	1.00	0.05	1,1,1,1	0
54	MG	BA	3037	1/1	1.00	0.06	0,0,0,0	0
54	MG	BA	3070	1/1	1.00	0.05	0,0,0,0	0
54	MG	BA	3013	1/1	1.00	0.09	0,0,0,0	0
54	MG	BA	3039	1/1	1.00	0.09	0,0,0,0	0
54	MG	BA	3040	1/1	1.00	0.03	2,2,2,2	0
54	MG	BA	3074	1/1	1.00	0.04	1,1,1,1	0
54	MG	BA	3123	1/1	1.00	0.07	0,0,0,0	0
54	MG	BA	3055	1/1	1.00	0.06	0,0,0,0	0
54	MG	BA	3041	1/1	1.00	0.03	2,2,2,2	0
54	MG	BA	3126	1/1	1.00	0.06	4,4,4,4	0
54	MG	BA	3014	1/1	1.00	0.05	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	ZN	B4	101	1/1	1.00	0.04	36,36,36,36	0
54	MG	CA	1625	1/1	1.00	0.10	17,17,17,17	0

5.5 Other polymers [i](#)

There are no such residues in this entry.