



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 01:44 AM UTC

PDB ID : 4U27 / pdb_00004u27
Title : Crystal structure of the E. coli ribosome bound to flopristin and linopristin.
Authors : Noeske, J.; Huang, J.; Olivier, N.B.; Giacobbe, R.A.; Zambrowski, M.; Cate, J.H.D.
Deposited on : 2014-07-16
Resolution : 2.80 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 : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.48.1

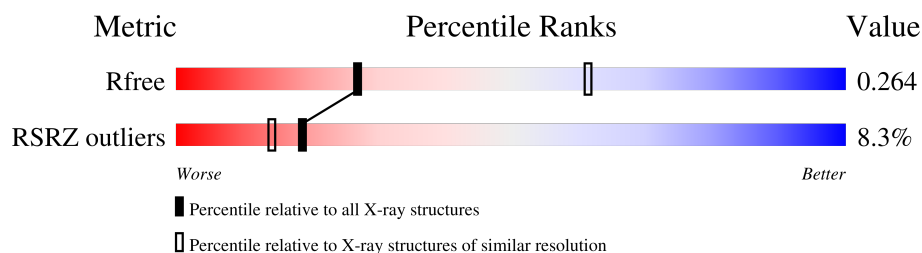
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	3657 (2.80-2.80)
RSRZ outliers	164620	3659 (2.80-2.80)

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	MHW	B6	1	-	X	-	-
54	MHW	D6	1	-	X	-	-
55	MG	BA	3137	-	-	-	X
55	MG	DA	3027	-	-	-	X
55	MG	DA	3062	-	-	-	X

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 288396 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 509	C 313	N 99	O 95	S 2	0	0	0
46	DY	63	Total 509	C 313	N 99	O 95	S 2	0	0	0

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

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

- 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			

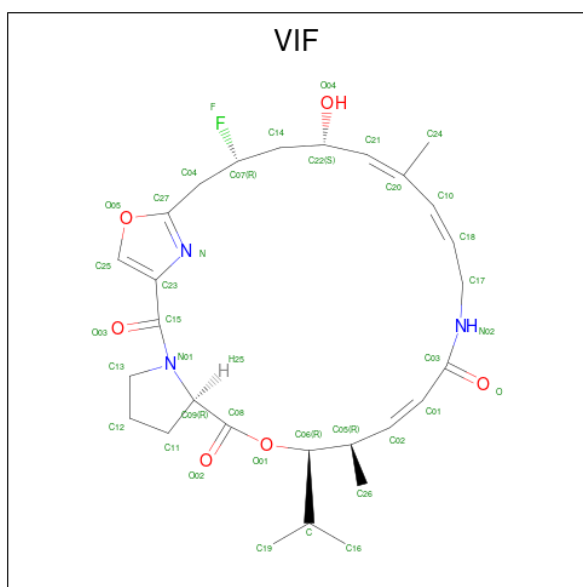
- Molecule 54 is a protein called Linopristin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
54	B6	7	Total	C	N	O	0	0	0
			69	50	9	10			
54	D6	7	Total	C	N	O	0	0	0
			69	50	9	10			

- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	AA	72	Total	Mg	0	0
			72	72		
55	BA	193	Total	Mg	0	0
			193	193		
55	BB	4	Total	Mg	0	0
			4	4		
55	BD	1	Total	Mg	0	0
			1	1		
55	BQ	1	Total	Mg	0	0
			1	1		
55	CA	56	Total	Mg	0	0
			56	56		
55	DA	167	Total	Mg	0	0
			167	167		
55	DB	3	Total	Mg	0	0
			3	3		
55	D2	1	Total	Mg	0	0
			1	1		

- Molecule 56 is Flopristin (CCD ID: VIF) (formula: C₂₈H₃₈FN₃O₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
56	BA	1	Total	C	F	N	O	0	0
			38	28	1	3	6		
56	DA	1	Total	C	F	N	O	0	0
			38	28	1	3	6		

- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 58 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	AA	193	Total	O	0	0
			193	193		
58	AL	2	Total	O	0	0
			2	2		
58	AN	5	Total	O	0	0
			5	5		
58	AT	2	Total	O	0	0
			2	2		
58	AU	1	Total	O	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	BA	623	Total O 623 623	0	0
58	BB	14	Total O 14 14	0	0
58	BC	6	Total O 6 6	0	0
58	BD	3	Total O 3 3	0	0
58	BE	4	Total O 4 4	0	0
58	BF	1	Total O 1 1	0	0
58	BG	1	Total O 1 1	0	0
58	BL	4	Total O 4 4	0	0
58	BN	3	Total O 3 3	0	0
58	BS	1	Total O 1 1	0	0
58	BT	1	Total O 1 1	0	0
58	B2	1	Total O 1 1	0	0
58	B3	2	Total O 2 2	0	0
58	B4	2	Total O 2 2	0	0
58	CA	192	Total O 192 192	0	0
58	CL	1	Total O 1 1	0	0
58	CN	3	Total O 3 3	0	0
58	CT	1	Total O 1 1	0	0
58	CU	1	Total O 1 1	0	0
58	DA	608	Total O 608 608	0	0
58	DB	13	Total O 13 13	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	DC	11	Total 11	O 11	0	0
58	DD	4	Total 4	O 4	0	0
58	DE	5	Total 5	O 5	0	0
58	DJ	1	Total 1	O 1	0	0
58	DL	4	Total 4	O 4	0	0
58	DN	2	Total 2	O 2	0	0
58	DT	1	Total 1	O 1	0	0
58	DU	1	Total 1	O 1	0	0
58	DV	1	Total 1	O 1	0	0
58	D0	1	Total 1	O 1	0	0
58	D2	1	Total 1	O 1	0	0
58	D3	2	Total 2	O 2	0	0
58	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	211.97Å 434.65Å 623.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	69.36 – 2.80 69.36 – 2.80	Depositor EDS
% Data completeness (in resolution range)	89.2 (69.36-2.80) 89.2 (69.36-2.80)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.215 , 0.260 0.220 , 0.264	Depositor DCC
R_{free} test set	5006 reflections (0.40%)	wwPDB-VP
Wilson B-factor (Å ²)	51.2	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 48.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	288396	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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](#)

10 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
54	MHW	B6	1	54	9,9,10	3.61	4 (44%)	10,11,13	2.83	6 (60%)
54	004	B6	7	54	9,10,11	4.39	7 (77%)	9,12,14	1.38	1 (11%)
54	04X	D6	6	54	14,16,17	1.19	1 (7%)	11,20,22	4.89	7 (63%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
54	04X	B6	6	54	14,16,17	1.48	1 (7%)	11,20,22	4.75	6 (54%)
54	MHU	D6	5	54	14,15,16	2.99	7 (50%)	18,19,21	2.56	2 (11%)
54	DBB	D6	3	54	4,5,6	0.67	0	1,5,7	1.85	0
54	MHU	B6	5	54	14,15,16	3.05	8 (57%)	18,19,21	2.92	5 (27%)
54	004	D6	7	54	9,10,11	3.71	7 (77%)	9,12,14	1.78	3 (33%)
54	MHW	D6	1	54	9,9,10	3.58	4 (44%)	10,11,13	2.58	6 (60%)
54	DBB	B6	3	54	4,5,6	0.38	0	1,5,7	1.34	0

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
54	MHW	B6	1	54	-	0/2/2/4	0/1/1/1
54	004	B6	7	54	-	0/4/6/8	0/1/1/1
54	04X	D6	6	54	-	3/5/24/26	0/2/2/2
54	04X	B6	6	54	-	2/5/24/26	0/2/2/2
54	MHU	D6	5	54	-	2/9/12/14	0/1/1/1
54	DBB	D6	3	54	-	1/3/4/6	-
54	MHU	B6	5	54	-	0/9/12/14	0/1/1/1
54	004	D6	7	54	-	1/4/6/8	0/1/1/1
54	MHW	D6	1	54	-	0/2/2/4	0/1/1/1
54	DBB	B6	3	54	-	0/3/4/6	-

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	B6	7	004	CB-CA	-9.04	1.43	1.52
54	B6	1	MHW	CA-N	-7.11	1.27	1.35
54	D6	1	MHW	CA-N	-6.91	1.27	1.35
54	B6	5	MHU	CE1-CD1	6.48	1.49	1.38
54	D6	5	MHU	CE1-CD1	6.35	1.49	1.38
54	D6	7	004	CB-CA	-6.02	1.46	1.52
54	D6	1	MHW	CG2-CB	-5.44	1.30	1.39
54	B6	1	MHW	CG2-CB	-5.44	1.30	1.39
54	B6	7	004	CG1-CB	-4.94	1.31	1.39
54	B6	6	04X	CE-N	-4.68	1.40	1.46
54	B6	5	MHU	CM-N	-4.58	1.35	1.46
54	D6	5	MHU	CD2-CG	4.51	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	D6	7	004	CD2-CE	4.43	1.48	1.38
54	B6	5	MHU	CD2-CG	4.28	1.47	1.38
54	D6	5	MHU	CM-N	-4.21	1.36	1.46
54	D6	1	MHW	CA-C	-4.21	1.44	1.48
54	B6	7	004	CD2-CE	4.18	1.47	1.38
54	D6	7	004	CG1-CB	-4.10	1.32	1.39
54	B6	1	MHW	CA-C	-4.03	1.44	1.48
54	D6	7	004	CD2-CG2	-3.91	1.32	1.38
54	B6	7	004	CD2-CG2	-3.87	1.32	1.38
54	B6	5	MHU	CE2-CZ	3.83	1.46	1.39
54	B6	7	004	CD1-CG1	3.83	1.45	1.38
54	D6	7	004	CD1-CG1	3.69	1.45	1.38
54	D6	5	MHU	CE2-CZ	3.39	1.45	1.39
54	D6	6	04X	CE-N	-3.34	1.42	1.46
54	B6	7	004	CD1-CE	-3.28	1.31	1.38
54	D6	7	004	CD1-CE	-3.26	1.31	1.38
54	B6	1	MHW	OG1-CB	3.24	1.42	1.36
54	D6	5	MHU	CD2-CE2	-3.13	1.33	1.38
54	B6	5	MHU	CD2-CE2	-3.00	1.34	1.38
54	D6	1	MHW	OG1-CB	2.96	1.42	1.36
54	D6	5	MHU	CE1-CZ	-2.83	1.33	1.39
54	D6	7	004	CA-C	-2.71	1.46	1.51
54	B6	5	MHU	CZ1-NZ	-2.68	1.39	1.45
54	B6	7	004	CA-C	-2.54	1.46	1.51
54	B6	5	MHU	CZ2-NZ	-2.34	1.40	1.45
54	D6	5	MHU	CZ1-NZ	-2.30	1.40	1.45
54	B6	5	MHU	CE1-CZ	-2.17	1.35	1.39

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	D6	6	04X	C0-N1-C1	13.70	132.45	111.14
54	B6	6	04X	C0-N1-C1	13.26	131.77	111.14
54	B6	5	MHU	CB-CA-N	8.24	122.61	110.48
54	D6	5	MHU	CB-CA-N	8.00	122.26	110.48
54	B6	5	MHU	O-C-CA	-7.21	106.23	124.77
54	D6	5	MHU	O-C-CA	-6.05	109.21	124.77
54	B6	1	MHW	CB-CA-C	-5.94	115.68	120.09
54	D6	6	04X	C2-C1-N1	-4.77	102.88	110.12
54	D6	1	MHW	CB-CA-C	-4.70	116.60	120.09
54	B6	6	04X	C0-N1-C4	-4.47	104.19	111.14
54	B6	6	04X	C2-C1-N1	-4.23	103.70	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	D6	6	04X	C3-O1-C2	3.50	121.21	109.88
54	D6	6	04X	C3-C4-N1	-3.43	104.91	110.12
54	B6	6	04X	C3-O1-C2	3.37	120.78	109.88
54	B6	6	04X	C4-N1-C1	3.37	116.11	108.84
54	D6	6	04X	C4-N1-C1	3.34	116.03	108.84
54	D6	7	004	CB-CA-C	3.12	120.85	112.09
54	B6	1	MHW	CD-CE-N	-3.11	118.49	123.42
54	B6	5	MHU	CB-CA-C	-3.03	105.78	111.81
54	D6	1	MHW	CB-CA-N	3.02	125.27	121.19
54	B6	1	MHW	OG1-CB-CG2	2.82	126.92	119.36
54	D6	1	MHW	CD-CE-N	-2.80	118.98	123.42
54	B6	7	004	CB-CA-C	2.77	119.86	112.09
54	D6	7	004	CG2-CB-CA	2.75	124.92	120.64
54	B6	5	MHU	CG-CB-CA	2.75	117.42	113.51
54	D6	1	MHW	OG1-CB-CG2	2.56	126.23	119.36
54	D6	1	MHW	O-C-CA	-2.55	121.17	124.37
54	B6	1	MHW	CB-CA-N	2.53	124.60	121.19
54	D6	6	04X	C0-N1-C4	-2.43	107.37	111.14
54	D6	1	MHW	CG2-CD-CE	2.39	122.38	118.92
54	B6	1	MHW	CG2-CD-CE	2.38	122.36	118.92
54	B6	6	04X	O1-C3-C4	-2.31	106.79	111.77
54	B6	1	MHW	O-C-CA	-2.27	121.53	124.37
54	D6	6	04X	O1-C2-C1	-2.12	107.20	111.77
54	B6	5	MHU	CE1-CZ-NZ	-2.10	118.84	121.65
54	D6	7	004	CG1-CB-CA	-2.07	117.42	120.64

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	D6	3	DBB	O-C-CA-CB
54	B6	6	04X	CD-C0-N1-C1
54	D6	6	04X	CD-C0-N1-C1
54	D6	6	04X	N1-C0-CD-CG
54	D6	5	MHU	CA-CB-CG-CD2
54	D6	5	MHU	CA-CB-CG-CD1
54	D6	6	04X	O-C-CA-CB
54	B6	6	04X	N1-C0-CD-CG
54	D6	7	004	N-CA-CB-CG2

There are no ring outliers.

No monomer is involved in short contacts.

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 502 ligands modelled in this entry, 500 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$
56	VIF	DA	3001	-	35,40,40	2.38	14 (40%)	43,55,55	2.32	13 (30%)
56	VIF	BA	3001	-	35,40,40	2.37	15 (42%)	43,55,55	2.16	14 (32%)

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
56	VIF	DA	3001	-	-	5/42/58/58	0/2/3/3
56	VIF	BA	3001	-	-	3/42/58/58	0/2/3/3

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	BA	3001	VIF	O01-C06	-4.81	1.37	1.44
56	DA	3001	VIF	O04-C22	-4.66	1.35	1.43
56	DA	3001	VIF	O01-C06	-4.56	1.38	1.44
56	BA	3001	VIF	O01-C08	-4.50	1.24	1.34
56	DA	3001	VIF	O01-C08	-4.43	1.24	1.34
56	BA	3001	VIF	C11-C09	-4.40	1.43	1.53
56	DA	3001	VIF	C15-N01	4.34	1.44	1.34
56	BA	3001	VIF	C03-N02	4.30	1.43	1.34
56	DA	3001	VIF	C11-C09	-4.25	1.43	1.53
56	BA	3001	VIF	C15-N01	3.79	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	BA	3001	VIF	O04-C22	-3.52	1.37	1.43
56	DA	3001	VIF	C03-N02	3.39	1.41	1.34
56	DA	3001	VIF	C09-N01	-3.34	1.40	1.47
56	BA	3001	VIF	C09-N01	-3.26	1.40	1.47
56	BA	3001	VIF	F-C07	-3.17	1.25	1.40
56	BA	3001	VIF	C09-C08	-3.04	1.46	1.52
56	DA	3001	VIF	F-C07	-2.97	1.26	1.40
56	DA	3001	VIF	C14-C22	-2.88	1.47	1.52
56	BA	3001	VIF	C26-C05	-2.69	1.46	1.53
56	DA	3001	VIF	C26-C05	-2.64	1.46	1.53
56	DA	3001	VIF	C23-N	-2.60	1.29	1.37
56	DA	3001	VIF	C09-C08	-2.59	1.47	1.52
56	BA	3001	VIF	C14-C22	-2.52	1.48	1.52
56	BA	3001	VIF	C13-N01	-2.40	1.43	1.47
56	BA	3001	VIF	C23-N	-2.28	1.30	1.37
56	DA	3001	VIF	C13-N01	-2.20	1.43	1.47
56	BA	3001	VIF	C12-C13	-2.14	1.44	1.51
56	DA	3001	VIF	C23-C15	-2.08	1.47	1.50
56	BA	3001	VIF	C16-C	-2.08	1.45	1.52

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	BA	3001	VIF	C02-C01-C03	-6.79	106.72	122.67
56	DA	3001	VIF	C02-C01-C03	-6.36	107.71	122.67
56	DA	3001	VIF	C14-C07-C04	-6.23	105.13	113.89
56	DA	3001	VIF	C18-C10-C20	-6.01	116.82	125.89
56	BA	3001	VIF	O01-C08-C09	4.61	120.38	110.80
56	BA	3001	VIF	C18-C10-C20	-4.27	119.44	125.89
56	DA	3001	VIF	O01-C08-C09	4.03	119.17	110.80
56	DA	3001	VIF	C06-O01-C08	3.99	124.39	117.76
56	BA	3001	VIF	C07-C14-C22	-3.62	108.39	114.25
56	BA	3001	VIF	C19-C-C16	-3.53	100.87	110.58
56	DA	3001	VIF	O01-C06-C05	3.52	112.94	107.12
56	BA	3001	VIF	C24-C20-C10	3.12	122.86	118.09
56	DA	3001	VIF	C19-C-C16	-2.99	102.36	110.58
56	BA	3001	VIF	O03-C15-N01	-2.94	116.90	121.62
56	DA	3001	VIF	C26-C05-C02	-2.91	103.32	109.91
56	DA	3001	VIF	C24-C20-C10	2.91	122.53	118.09
56	BA	3001	VIF	O01-C08-O02	-2.76	118.96	123.95
56	BA	3001	VIF	C26-C05-C02	-2.72	103.75	109.91
56	BA	3001	VIF	C10-C20-C21	-2.70	111.59	118.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	BA	3001	VIF	C06-O01-C08	2.47	121.86	117.76
56	BA	3001	VIF	C26-C05-C06	2.45	115.42	111.11
56	DA	3001	VIF	C06-C05-C02	2.44	117.22	109.46
56	DA	3001	VIF	C10-C20-C21	-2.43	112.31	118.82
56	DA	3001	VIF	O01-C08-O02	-2.39	119.63	123.95
56	DA	3001	VIF	C26-C05-C06	2.38	115.30	111.11
56	BA	3001	VIF	C01-C03-N02	2.23	119.95	115.07
56	BA	3001	VIF	O-C03-N02	-2.06	119.06	122.29

There are no chirality outliers.

All (8) torsion outliers are listed below:

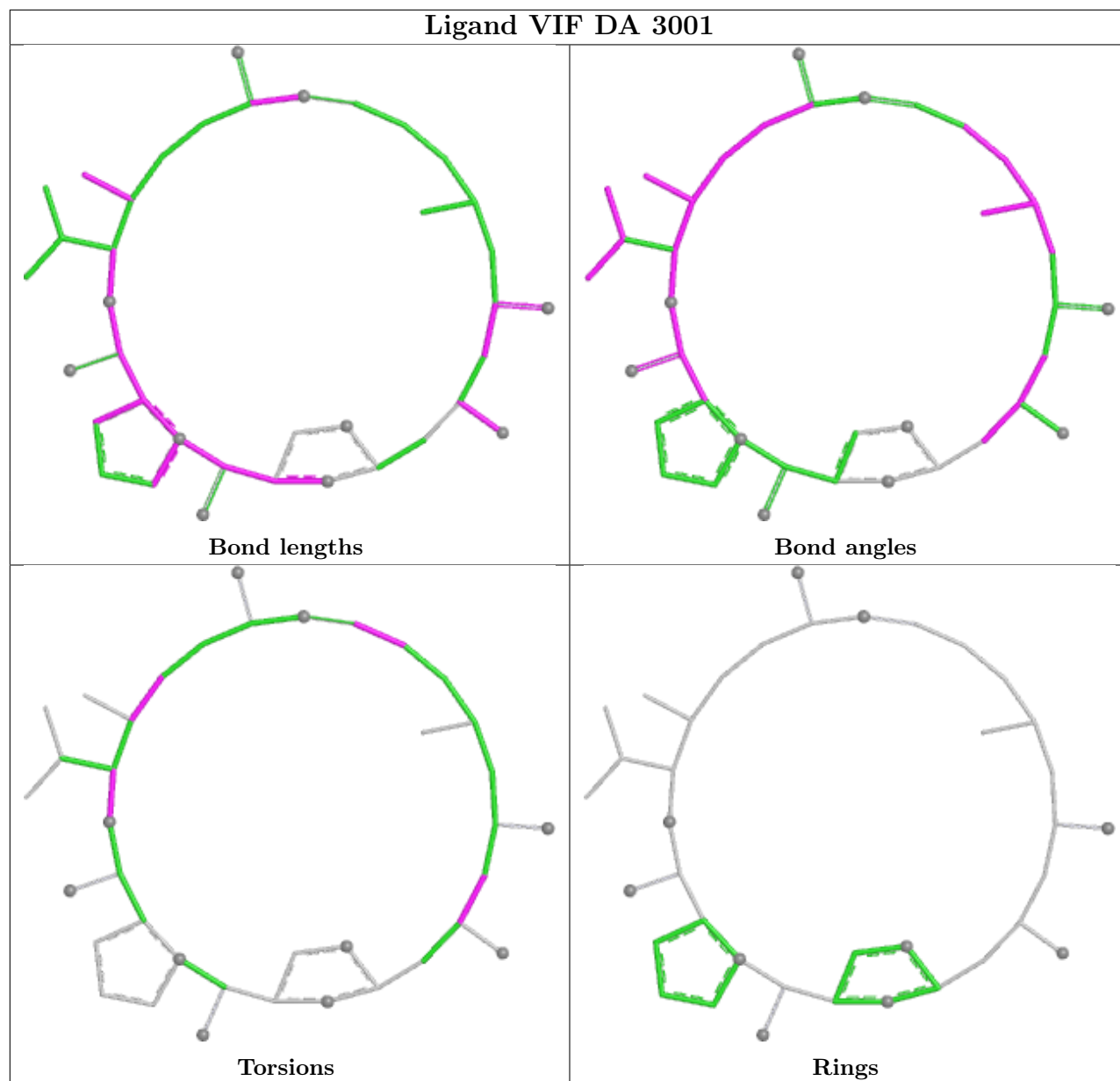
Mol	Chain	Res	Type	Atoms
56	DA	3001	VIF	F-C07-C14-C22
56	BA	3001	VIF	C02-C01-C03-O
56	BA	3001	VIF	C02-C01-C03-N02
56	DA	3001	VIF	C05-C06-O01-C08
56	DA	3001	VIF	C-C06-O01-C08
56	BA	3001	VIF	C01-C02-C05-C26
56	DA	3001	VIF	N02-C17-C18-C10
56	DA	3001	VIF	C01-C02-C05-C26

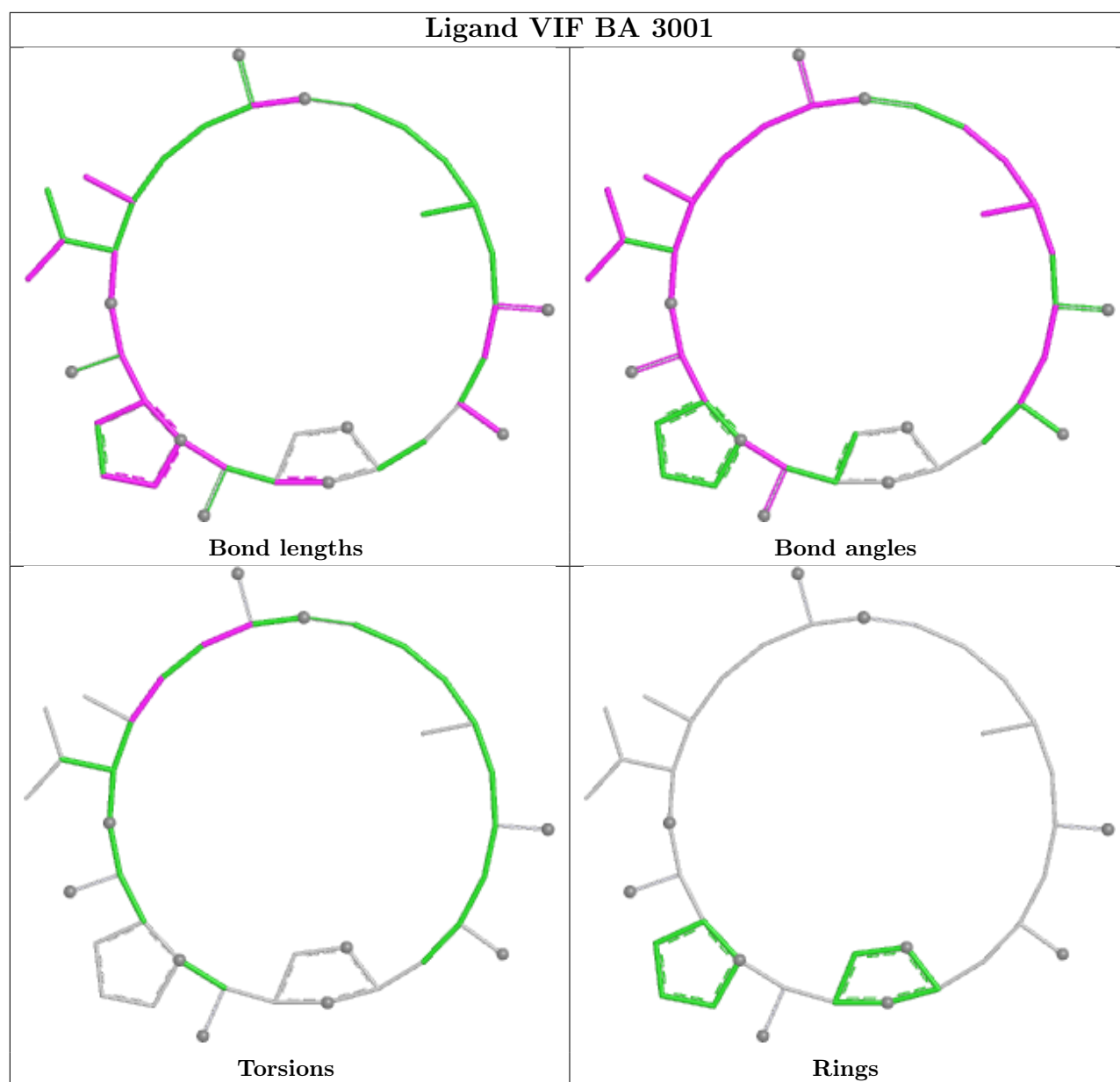
There are no ring outliers.

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.

Ligand VIF DA 3001





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%)	-0.14	32 (2%) 63 55	13, 50, 135, 180	0
1	CA	1539/1539 (100%)	0.36	67 (4%) 39 32	27, 70, 145, 177	0
2	AB	218/218 (100%)	0.51	12 (5%) 32 25	38, 73, 99, 121	0
2	CB	218/218 (100%)	0.92	25 (11%) 11 9	61, 87, 107, 125	0
3	AC	206/206 (100%)	-0.03	5 (2%) 59 51	33, 57, 78, 93	0
3	CC	206/206 (100%)	0.54	10 (4%) 36 28	48, 78, 95, 105	0
4	AD	205/205 (100%)	0.20	9 (4%) 39 32	32, 55, 79, 105	0
4	CD	205/205 (100%)	-0.03	10 (4%) 36 28	18, 38, 64, 88	0
5	AE	150/150 (100%)	0.08	5 (3%) 49 41	30, 48, 79, 102	0
5	CE	150/150 (100%)	0.35	8 (5%) 33 26	32, 56, 82, 104	0
6	AF	100/100 (100%)	0.10	2 (2%) 64 56	34, 58, 73, 86	0
6	CF	100/100 (100%)	0.43	6 (6%) 29 22	44, 74, 93, 105	0
7	AG	151/151 (100%)	0.34	7 (4%) 38 30	54, 77, 96, 102	0
7	CG	151/151 (100%)	1.57	42 (27%) 2 2	81, 100, 109, 114	0
8	AH	129/129 (100%)	-0.13	2 (1%) 70 63	27, 48, 66, 76	0
8	CH	129/129 (100%)	0.27	4 (3%) 51 43	49, 65, 80, 90	0
9	AI	127/127 (100%)	0.75	14 (11%) 12 9	43, 73, 96, 109	0
9	CI	127/127 (100%)	1.27	23 (18%) 4 4	71, 93, 110, 122	0
10	AJ	98/98 (100%)	0.73	10 (10%) 13 10	40, 64, 92, 122	0
10	CJ	98/98 (100%)	1.38	25 (25%) 2 2	72, 93, 111, 125	0
11	AK	117/117 (100%)	0.37	4 (3%) 48 40	27, 65, 91, 115	0
11	CK	117/117 (100%)	0.07	3 (2%) 57 49	39, 66, 79, 93	0
12	AL	123/123 (100%)	-0.03	6 (4%) 36 28	18, 35, 64, 96	0
12	CL	123/123 (100%)	0.45	8 (6%) 26 20	38, 52, 78, 98	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	114/114 (100%)	0.23	3 (2%) 57 49	45, 68, 92, 102	0
13	CM	114/114 (100%)	1.95	54 (47%) 0 1	96, 108, 116, 119	0
14	AN	96/100 (96%)	0.70	12 (12%) 9 8	37, 58, 94, 103	0
14	CN	96/100 (96%)	1.36	25 (26%) 2 2	69, 94, 111, 120	0
15	AO	88/88 (100%)	0.18	2 (2%) 61 52	28, 51, 65, 90	0
15	CO	88/88 (100%)	0.13	1 (1%) 77 71	40, 62, 80, 98	0
16	AP	82/82 (100%)	0.33	7 (8%) 18 14	31, 47, 85, 101	0
16	CP	82/82 (100%)	0.64	3 (3%) 45 37	44, 61, 87, 105	0
17	AQ	80/80 (100%)	0.36	4 (5%) 35 28	27, 49, 77, 122	0
17	CQ	80/80 (100%)	0.93	9 (11%) 11 9	44, 75, 97, 102	0
18	AR	55/55 (100%)	-0.06	1 (1%) 67 60	39, 52, 78, 108	0
18	CR	55/55 (100%)	0.23	3 (5%) 32 25	42, 55, 79, 111	0
19	AS	79/79 (100%)	0.54	7 (8%) 17 13	52, 68, 89, 102	0
19	CS	79/79 (100%)	2.10	41 (51%) 0 0	89, 108, 118, 124	0
20	AT	85/85 (100%)	0.22	5 (5%) 29 22	34, 48, 70, 103	0
20	CT	85/85 (100%)	0.99	11 (12%) 9 7	55, 73, 91, 97	0
21	AU	51/51 (100%)	1.51	14 (27%) 2 2	48, 74, 95, 106	0
21	CU	51/51 (100%)	1.28	12 (23%) 2 3	45, 71, 96, 105	0
22	BA	2897/2903 (99%)	-0.60	131 (4%) 39 31	0, 13, 130, 195	0
22	DA	2897/2903 (99%)	0.76	160 (5%) 32 25	40, 82, 145, 181	0
23	BB	119/119 (100%)	-0.80	1 (0%) 82 77	2, 23, 49, 85	0
23	DB	118/119 (99%)	0.77	3 (2%) 58 49	66, 112, 133, 143	0
24	BC	271/271 (100%)	-0.56	3 (1%) 77 71	3, 19, 36, 51	0
24	DC	271/271 (100%)	0.71	28 (10%) 13 10	43, 61, 77, 89	0
25	BD	209/209 (100%)	-0.85	0 100 100	0, 10, 34, 68	0
25	DD	209/209 (100%)	0.91	28 (13%) 8 7	49, 68, 83, 96	0
26	BE	201/201 (100%)	-0.60	1 (0%) 87 83	1, 23, 54, 90	0
26	DE	201/201 (100%)	1.36	43 (21%) 3 3	42, 84, 100, 108	0
27	BF	177/177 (100%)	-0.16	1 (0%) 85 81	20, 41, 78, 90	0
27	DF	177/177 (100%)	1.21	24 (13%) 8 7	90, 107, 119, 125	0
28	BG	176/176 (100%)	-0.37	1 (0%) 85 81	17, 37, 62, 84	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DG	176/176 (100%)	1.11	27 (15%) 6 5	72, 93, 105, 114	0
29	BH	149/149 (100%)	2.32	81 (54%) 0 0	25, 102, 121, 129	0
29	DH	149/149 (100%)	1.41	34 (22%) 2 3	25, 92, 107, 115	0
30	BI	141/141 (100%)	1.89	61 (43%) 1 1	90, 111, 122, 133	0
30	DI	141/141 (100%)	2.56	82 (58%) 0 0	101, 117, 127, 130	0
31	BJ	142/142 (100%)	-0.84	0 100 100	1, 6, 22, 36	0
31	DJ	142/142 (100%)	0.70	20 (14%) 7 6	50, 66, 79, 96	0
32	BK	122/122 (100%)	-0.75	2 (1%) 70 63	4, 12, 32, 67	0
32	DK	122/122 (100%)	0.53	10 (8%) 19 14	46, 63, 82, 97	0
33	BL	143/143 (100%)	-0.49	1 (0%) 84 79	1, 18, 43, 74	0
33	DL	143/143 (100%)	1.33	32 (22%) 3 3	46, 79, 94, 113	0
34	BM	136/136 (100%)	-0.81	1 (0%) 84 79	1, 9, 29, 84	0
34	DM	136/136 (100%)	0.53	6 (4%) 39 32	45, 69, 82, 101	0
35	BN	120/120 (100%)	-0.86	0 100 100	2, 7, 16, 52	0
35	DN	120/120 (100%)	1.28	19 (15%) 6 5	56, 75, 88, 114	0
36	BO	116/116 (100%)	-0.53	0 100 100	13, 24, 42, 50	0
36	DO	116/116 (100%)	0.92	12 (10%) 13 10	80, 94, 105, 114	0
37	BP	114/114 (100%)	-0.66	0 100 100	6, 18, 42, 64	0
37	DP	114/114 (100%)	0.68	4 (3%) 47 39	57, 69, 86, 91	0
38	BQ	117/117 (100%)	-0.84	0 100 100	1, 4, 13, 31	0
38	DQ	117/117 (100%)	0.94	19 (16%) 5 5	52, 67, 78, 82	0
39	BR	103/103 (100%)	-0.63	1 (0%) 79 73	0, 11, 33, 66	0
39	DR	103/103 (100%)	1.00	12 (11%) 10 9	51, 77, 88, 99	0
40	BS	110/110 (100%)	-0.82	1 (0%) 81 75	1, 4, 21, 80	0
40	DS	110/110 (100%)	1.21	23 (20%) 3 3	57, 74, 89, 100	0
41	BT	93/93 (100%)	-0.30	6 (6%) 26 20	8, 26, 75, 103	0
41	DT	93/93 (100%)	1.82	37 (39%) 1 1	66, 85, 103, 117	0
42	BU	102/102 (100%)	-0.45	0 100 100	12, 28, 63, 92	0
42	DU	102/102 (100%)	1.99	44 (43%) 1 1	75, 90, 109, 118	0
43	BV	94/94 (100%)	-0.79	0 100 100	5, 19, 41, 53	0
43	DV	94/94 (100%)	0.59	4 (4%) 40 32	69, 84, 95, 104	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BW	76/76 (100%)	-0.68	1 (1%) 74 67	4, 12, 27, 54	0
44	DW	75/76 (98%)	1.05	11 (14%) 7 6	60, 80, 90, 105	0
45	BX	77/77 (100%)	-0.40	1 (1%) 74 67	6, 24, 51, 73	0
45	DX	77/77 (100%)	1.24	16 (20%) 3 3	51, 71, 84, 87	0
46	BY	63/63 (100%)	0.03	3 (4%) 36 29	20, 40, 73, 93	0
46	DY	63/63 (100%)	1.42	15 (23%) 2 3	78, 94, 100, 105	0
47	BZ	58/58 (100%)	-0.77	0 100 100	2, 6, 23, 42	0
47	DZ	58/58 (100%)	0.84	6 (10%) 13 10	58, 71, 81, 94	0
48	B0	56/56 (100%)	-0.78	0 100 100	0, 9, 36, 68	0
48	D0	56/56 (100%)	1.13	9 (16%) 5 5	56, 78, 92, 102	0
49	B1	50/50 (100%)	-0.50	1 (2%) 64 56	17, 29, 49, 77	0
49	D1	50/50 (100%)	1.19	9 (18%) 4 4	69, 84, 93, 103	0
50	B2	46/46 (100%)	-0.69	1 (2%) 62 53	3, 9, 16, 88	0
50	D2	46/46 (100%)	1.50	13 (28%) 1 2	56, 68, 79, 102	0
51	B3	64/64 (100%)	-0.77	0 100 100	4, 9, 16, 31	0
51	D3	64/64 (100%)	1.56	20 (31%) 1 1	57, 71, 80, 81	0
52	B4	38/38 (100%)	-0.69	0 100 100	8, 16, 35, 52	0
52	D4	38/38 (100%)	1.39	9 (23%) 2 3	58, 75, 87, 101	0
53	B5	191/228 (83%)	2.16	95 (49%) 0 1	99, 115, 127, 135	0
54	B6	2/7 (28%)	-0.92	0 100 100	1, 1, 1, 1	0
54	D6	2/7 (28%)	0.91	1 (50%) 0 1	47, 47, 47, 57	0
All	All	20738/20808 (99%)	0.31	1727 (8%) 19 14	0, 62, 120, 195	0

All (1727) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
30	BI	53	LEU	11.3
29	BH	146	VAL	8.8
42	DU	58	ILE	8.6
9	CI	128	SER	8.4
30	DI	10	LYS	7.4
17	AQ	20	SER	7.2
7	CG	62	PHE	7.1
20	AT	68	HIS	6.8
29	BH	120	GLY	6.7

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Mol	Chain	Res	Type	RSRZ
22	BA	2189	U	6.6
11	CK	126	LYS	6.5
4	CD	25	VAL	6.5
29	DH	12	LEU	6.4
30	DI	11	LEU	6.4
29	BH	119	ASN	6.3
30	DI	54	PRO	6.3
30	DI	53	LEU	6.3
10	AJ	102	LEU	6.2
29	BH	121	VAL	6.1
30	DI	82	LYS	6.0
53	B5	216	THR	5.9
30	DI	83	ALA	5.8
30	DI	59	ILE	5.8
22	BA	1072	C	5.8
41	DT	76	ARG	5.7
2	AB	155	GLY	5.7
2	AB	157	LEU	5.6
22	BA	1926	U	5.6
30	DI	14	ALA	5.6
9	CI	20	PHE	5.6
30	DI	78	VAL	5.6
30	DI	58	VAL	5.5
33	DL	34	GLY	5.5
42	DU	12	ILE	5.5
21	AU	38	TYR	5.5
29	BH	81	ALA	5.5
30	DI	13	VAL	5.4
22	BA	2144	G	5.4
8	AH	2	SER	5.4
4	CD	24	GLY	5.4
22	BA	2185	U	5.4
2	AB	156	GLY	5.3
36	DO	2	ASP	5.3
20	CT	4	ILE	5.3
22	BA	2145	C	5.3
29	BH	67	ALA	5.3
29	BH	122	LEU	5.2
41	DT	36	LYS	5.2
50	D2	46	LYS	5.2
3	AC	193	TYR	5.2
9	CI	129	LYS	5.2

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Mol	Chain	Res	Type	RSRZ
41	DT	9	LYS	5.2
22	BA	1923	U	5.2
10	CJ	77	VAL	5.1
53	B5	76	LEU	5.1
1	AA	121	U	5.1
2	CB	135	LEU	5.0
22	BA	2152	G	5.0
42	DU	71	ALA	5.0
51	D3	37	ALA	5.0
13	CM	24	GLY	5.0
30	BI	81	LYS	5.0
29	BH	130	VAL	5.0
22	BA	2158	A	5.0
38	DQ	15	LYS	4.9
22	BA	2098	U	4.9
30	DI	129	ILE	4.9
22	BA	2885	G	4.9
29	BH	97	ARG	4.9
40	DS	84	ARG	4.9
29	BH	117	LEU	4.9
41	DT	57	VAL	4.9
1	AA	1535	C	4.9
1	CA	1302	C	4.9
53	B5	132	LEU	4.9
22	BA	2184	A	4.9
22	BA	2190	G	4.8
27	DF	54	ALA	4.8
30	BI	79	LEU	4.8
30	DI	9	VAL	4.8
53	B5	50	ILE	4.8
13	CM	27	LYS	4.8
22	BA	2157	G	4.8
14	CN	34	VAL	4.8
35	DN	25	ALA	4.8
13	CM	13	LYS	4.8
1	AA	1538	C	4.8
29	BH	69	ALA	4.7
30	BI	80	LEU	4.7
22	BA	2193	G	4.7
42	DU	13	VAL	4.7
30	DI	68	THR	4.7
3	AC	2	GLY	4.7

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Mol	Chain	Res	Type	RSRZ
22	BA	2174	C	4.7
29	BH	118	PRO	4.7
6	CF	91	ARG	4.7
21	CU	35	ARG	4.7
30	BI	27	ALA	4.7
16	AP	81	ALA	4.6
22	BA	2096	C	4.6
9	AI	40	GLY	4.6
24	DC	254	GLY	4.6
2	CB	164	ILE	4.6
13	CM	18	ALA	4.6
42	DU	43	LYS	4.6
9	CI	130	ARG	4.6
8	CH	3	MET	4.6
29	BH	63	ALA	4.6
53	B5	111	PHE	4.5
27	DF	79	ILE	4.5
29	BH	84	ALA	4.5
29	DH	58	LEU	4.5
19	CS	71	LEU	4.5
10	CJ	41	PRO	4.5
7	CG	75	VAL	4.5
35	DN	48	VAL	4.5
14	CN	57	PRO	4.5
53	B5	110	ASP	4.5
29	BH	91	PHE	4.4
38	DQ	11	ARG	4.4
42	DU	26	LYS	4.4
50	D2	25	LYS	4.4
53	B5	217	THR	4.4
22	BA	2175	C	4.4
30	BI	11	LEU	4.4
30	DI	79	LEU	4.4
26	DE	42	GLY	4.4
29	BH	94	ILE	4.4
41	DT	34	VAL	4.4
29	BH	96	THR	4.4
24	DC	205	LEU	4.4
21	CU	45	ARG	4.4
1	CA	1535	C	4.4
22	DA	1093	G	4.3
30	DI	56	PRO	4.3

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Mol	Chain	Res	Type	RSRZ
12	AL	124	ALA	4.3
33	DL	15	ALA	4.3
13	CM	89	LEU	4.3
45	DX	3	ARG	4.3
24	DC	235	GLY	4.3
32	DK	68	GLY	4.3
2	CB	129	LEU	4.3
33	DL	27	LEU	4.3
42	DU	55	PRO	4.3
20	AT	4	ILE	4.3
31	DJ	47	HIS	4.3
4	AD	37	ALA	4.3
5	CE	157	ARG	4.3
38	DQ	2	ALA	4.3
53	B5	108	TRP	4.3
21	AU	53	VAL	4.2
53	B5	23	ILE	4.2
29	BH	108	VAL	4.2
22	BA	2147	A	4.2
50	B2	46	LYS	4.2
1	CA	1536	C	4.2
19	CS	38	SER	4.2
24	DC	92	ALA	4.2
38	DQ	8	VAL	4.2
35	DN	28	LEU	4.2
22	BA	2112	G	4.2
9	AI	43	THR	4.2
22	BA	1094	U	4.2
30	DI	3	LYS	4.2
33	DL	61	LEU	4.2
30	DI	109	ILE	4.2
53	B5	205	ALA	4.2
22	BA	2100	G	4.1
30	DI	7	ALA	4.1
42	DU	67	VAL	4.1
16	AP	80	LYS	4.1
42	DU	32	GLY	4.1
12	CL	38	TYR	4.1
38	DQ	9	ILE	4.1
21	AU	32	VAL	4.1
26	DE	33	VAL	4.1
30	DI	27	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
53	B5	87	ALA	4.1
2	CB	132	LYS	4.1
27	DF	88	LYS	4.1
45	DX	49	LEU	4.1
19	CS	78	ARG	4.1
29	BH	110	VAL	4.1
53	B5	120	VAL	4.1
22	DA	2149	U	4.1
22	BA	1847	A	4.0
1	CA	1032	G	4.0
29	BH	72	ILE	4.0
9	CI	64	TYR	4.0
19	CS	80	TYR	4.0
29	BH	115	VAL	4.0
30	DI	57	VAL	4.0
4	CD	27	ALA	4.0
22	BA	2104	C	4.0
14	AN	21	PHE	4.0
29	BH	144	VAL	4.0
42	DU	39	ILE	4.0
29	BH	124	THR	4.0
30	DI	60	THR	4.0
12	CL	25	GLU	4.0
38	DQ	29	SER	4.0
32	BK	35	VAL	4.0
22	BA	2140	G	4.0
21	AU	14	VAL	4.0
22	DA	1278	C	4.0
30	DI	5	VAL	4.0
42	DU	80	ALA	4.0
28	DG	9	VAL	3.9
29	DH	61	VAL	3.9
53	B5	73	VAL	3.9
14	AN	55	SER	3.9
22	BA	1924	C	3.9
13	CM	63	PHE	3.9
22	BA	2114	A	3.9
31	DJ	81	ILE	3.9
30	DI	38	PHE	3.9
7	AG	8	GLY	3.9
19	CS	72	GLY	3.9
22	BA	2130	U	3.9

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Mol	Chain	Res	Type	RSRZ
7	CG	87	VAL	3.9
19	CS	76	PRO	3.9
2	CB	151	ILE	3.9
53	B5	78	ILE	3.9
25	DD	157	LYS	3.9
49	D1	53	LYS	3.9
30	BI	2	ALA	3.9
26	DE	164	LEU	3.9
50	D2	42	LEU	3.9
26	DE	175	ILE	3.9
35	DN	97	ILE	3.9
22	BA	2156	G	3.9
42	DU	57	GLY	3.9
29	BH	148	ALA	3.9
13	CM	86	TYR	3.9
30	DI	42	PHE	3.9
31	DJ	119	PHE	3.9
1	CA	1331	G	3.9
30	DI	70	VAL	3.8
53	B5	62	THR	3.8
19	CS	14	HIS	3.8
22	BA	2135	A	3.8
44	DW	62	LYS	3.8
18	CR	20	GLU	3.8
39	DR	55	ASP	3.8
53	B5	106	ASP	3.8
22	BA	2159	G	3.8
30	DI	22	PRO	3.8
30	DI	74	PRO	3.8
32	DK	81	GLY	3.8
19	CS	60	VAL	3.8
30	DI	28	LEU	3.8
29	BH	56	ALA	3.8
53	B5	79	ALA	3.8
13	CM	98	ARG	3.8
26	DE	119	ILE	3.8
1	AA	1018	G	3.8
22	BA	1925	C	3.8
22	BA	2133	G	3.8
22	DA	331	C	3.8
22	BA	2169	A	3.8
7	CG	66	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
29	DH	15	LEU	3.8
29	BH	111	ALA	3.8
13	CM	45	ILE	3.8
22	BA	2099	U	3.8
26	DE	153	LEU	3.8
27	DF	66	LEU	3.8
46	DY	22	LEU	3.8
21	CU	53	VAL	3.7
40	DS	36	LEU	3.7
25	DD	154	LYS	3.7
5	CE	110	ALA	3.7
22	DA	654	A	3.7
30	DI	15	ALA	3.7
22	BA	2138	G	3.7
26	DE	131	THR	3.7
46	DY	19	LEU	3.7
10	CJ	57	VAL	3.7
3	CC	79	LYS	3.7
30	DI	81	LYS	3.7
7	CG	152	ALA	3.7
29	BH	106	ALA	3.7
31	DJ	118	MET	3.7
29	BH	70	GLU	3.7
35	DN	27	SER	3.7
1	AA	1534	A	3.7
1	CA	994	A	3.7
44	DW	52	GLY	3.7
19	AS	5	LEU	3.7
51	D3	44	LEU	3.7
7	CG	73	VAL	3.7
13	CM	43	VAL	3.7
22	BA	2113	U	3.7
35	DN	24	MET	3.7
30	DI	86	ILE	3.7
1	CA	1539	C	3.7
5	CE	158	GLY	3.7
29	BH	88	GLY	3.7
53	B5	133	GLY	3.7
21	AU	28	VAL	3.7
29	BH	98	ASP	3.7
29	BH	147	VAL	3.7
41	DT	55	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
21	CU	38	TYR	3.7
4	AD	28	ILE	3.7
19	CS	9	PRO	3.6
14	CN	48	LEU	3.6
11	AK	126	LYS	3.6
21	CU	14	VAL	3.6
2	CB	139	ARG	3.6
17	AQ	5	ILE	3.6
27	DF	67	ILE	3.6
20	CT	68	HIS	3.6
22	BA	2136	G	3.6
7	CG	118	LEU	3.6
7	CG	6	VAL	3.6
41	DT	73	ARG	3.6
29	BH	102	ALA	3.6
29	DH	47	PHE	3.6
14	CN	51	LEU	3.6
24	DC	18	LYS	3.6
53	B5	145	THR	3.6
29	BH	85	GLY	3.6
1	CA	1312	G	3.6
22	BA	2102	G	3.6
42	DU	59	VAL	3.6
19	CS	42	PRO	3.6
22	BA	2101	A	3.6
22	DA	76	C	3.6
29	BH	75	LEU	3.6
25	DD	170	VAL	3.6
30	DI	61	VAL	3.6
45	DX	4	VAL	3.6
20	CT	38	ALA	3.6
22	BA	2168	G	3.6
30	BI	67	PHE	3.6
30	DI	75	PRO	3.6
3	CC	33	LEU	3.6
29	DH	122	LEU	3.6
33	DL	19	LEU	3.6
53	B5	121	MET	3.5
2	CB	13	GLY	3.5
41	DT	71	GLY	3.5
53	B5	107	GLY	3.5
30	BI	77	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
2	CB	213	TYR	3.5
13	CM	31	LYS	3.5
30	DI	4	LYS	3.5
41	DT	81	LYS	3.5
22	DA	101	A	3.5
46	BY	23	ARG	3.5
13	CM	28	THR	3.5
16	CP	3	THR	3.5
9	CI	21	ILE	3.5
30	DI	101	ILE	3.5
1	CA	1031	C	3.5
53	B5	137	LEU	3.5
25	DD	111	GLY	3.5
1	AA	78	A	3.5
1	CA	1305	G	3.5
19	CS	39	THR	3.5
22	BA	2097	A	3.5
22	BA	2141	G	3.5
22	BA	2191	A	3.5
25	DD	139	SER	3.5
29	BH	131	SER	3.5
30	DI	2	ALA	3.5
42	DU	44	LYS	3.5
19	CS	41	PHE	3.5
22	BA	2143	C	3.5
22	BA	2165	C	3.5
22	DA	1606	C	3.5
30	BI	54	PRO	3.5
53	B5	140	ASN	3.5
53	B5	202	PRO	3.5
29	BH	90	LEU	3.5
26	DE	165	HIS	3.5
9	CI	112	GLU	3.5
26	DE	73	ILE	3.5
53	B5	218	THR	3.5
22	BA	2402	U	3.5
7	CG	103	TRP	3.5
29	BH	52	ALA	3.5
30	DI	44	ALA	3.5
22	DA	329	G	3.5
29	BH	62	LEU	3.5
42	DU	48	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
45	DX	35	SER	3.5
2	CB	136	MET	3.5
46	DY	48	ARG	3.5
44	DW	71	VAL	3.4
13	CM	22	ILE	3.4
40	DS	37	THR	3.4
14	AN	36	ALA	3.4
29	BH	74	ALA	3.4
33	DL	57	LEU	3.4
42	DU	82	ARG	3.4
22	BA	1087	G	3.4
22	BA	2103	C	3.4
14	CN	19	LYS	3.4
28	DG	6	LYS	3.4
42	DU	3	ALA	3.4
22	BA	2142	A	3.4
22	BA	2176	A	3.4
10	AJ	74	VAL	3.4
38	DQ	39	VAL	3.4
10	CJ	76	ILE	3.4
25	DD	153	GLY	3.4
22	BA	1922	G	3.4
22	BA	2123	G	3.4
22	DA	1537	G	3.4
20	CT	72	ALA	3.4
30	DI	76	ALA	3.4
50	D2	1	MET	3.4
53	B5	187	ALA	3.4
17	AQ	83	VAL	3.4
30	BI	63	ALA	3.4
1	CA	1132	C	3.4
22	BA	1071	G	3.4
22	BA	2148	G	3.4
6	CF	79	ARG	3.4
28	DG	62	TRP	3.4
46	DY	47	ARG	3.4
20	CT	33	LYS	3.4
24	DC	104	ILE	3.4
36	DO	4	LYS	3.4
51	D3	15	LYS	3.4
30	BI	52	GLY	3.4
10	CJ	102	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
22	BA	715	A	3.3
22	DA	1073	A	3.3
29	DH	54	LEU	3.3
51	D3	24	HIS	3.3
30	DI	55	ILE	3.3
53	B5	84	ILE	3.3
4	AD	24	GLY	3.3
10	AJ	87	LEU	3.3
19	CS	15	LEU	3.3
53	B5	109	MET	3.3
22	DA	332	A	3.3
30	BI	14	ALA	3.3
9	AI	41	ARG	3.3
15	AO	89	ARG	3.3
19	AS	56	GLN	3.3
34	DM	8	LYS	3.3
33	BL	115	GLU	3.3
33	DL	106	GLU	3.3
35	DN	26	GLY	3.3
46	DY	59	GLU	3.3
30	DI	106	LEU	3.3
53	B5	166	ASN	3.3
22	DA	325	G	3.3
22	DA	504	A	3.3
22	DA	2126	A	3.3
25	DD	96	ILE	3.3
27	DF	106	ILE	3.3
52	D4	3	VAL	3.3
29	BH	114	GLU	3.3
30	DI	80	LEU	3.3
45	DX	22	LEU	3.3
22	BA	2182	U	3.3
20	AT	36	TYR	3.3
13	CM	29	ARG	3.3
53	B5	77	ALA	3.3
22	BA	1171	G	3.3
36	DO	58	ILE	3.3
2	CB	92	VAL	3.3
1	AA	1492	A	3.3
13	CM	94	GLY	3.3
38	DQ	23	GLY	3.3
30	BI	38	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
22	DA	2402	U	3.2
30	BI	128	SER	3.2
33	DL	58	TYR	3.2
7	CG	78	ARG	3.2
22	BA	2164	C	3.2
22	DA	2008	C	3.2
2	CB	207	ILE	3.2
41	BT	2	ILE	3.2
2	AB	104	TRP	3.2
3	AC	175	LEU	3.2
22	DA	333	G	3.2
1	CA	1145	A	3.2
21	CU	47	ARG	3.2
30	BI	23	PRO	3.2
9	AI	44	ALA	3.2
28	DG	157	TYR	3.2
29	BH	140	ALA	3.2
22	DA	846	U	3.2
22	DA	2172	U	3.2
40	DS	83	LYS	3.2
40	DS	96	ILE	3.2
7	CG	72	THR	3.2
30	BI	24	VAL	3.2
30	DI	118	THR	3.2
53	B5	35	THR	3.2
22	BA	2178	C	3.2
21	CU	16	LEU	3.2
13	CM	99	GLY	3.2
29	BH	129	GLU	3.2
22	BA	1062	G	3.2
22	BA	2134	A	3.2
29	BH	71	LYS	3.2
29	BH	123	ARG	3.2
53	B5	165	ARG	3.2
3	CC	193	TYR	3.2
12	AL	38	TYR	3.2
29	BH	73	ASN	3.2
19	CS	45	ILE	3.2
22	BA	2122	U	3.2
29	BH	99	ILE	3.2
49	D1	48	ILE	3.2
33	DL	89	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
9	CI	66	THR	3.2
49	D1	36	LEU	3.2
1	CA	995	C	3.2
22	DA	680	C	3.2
31	DJ	9	GLU	3.2
30	BI	82	LYS	3.2
26	DE	36	ALA	3.2
17	CQ	21	ILE	3.2
30	BI	86	ILE	3.2
30	DI	122	ILE	3.2
1	CA	94	G	3.2
1	CA	1033	G	3.2
22	BA	2188	U	3.2
30	BI	135	SER	3.2
30	DI	98	VAL	3.2
36	DO	103	VAL	3.2
30	BI	68	THR	3.2
19	CS	68	GLY	3.2
41	DT	68	LYS	3.2
44	DW	60	PHE	3.2
22	BA	885	C	3.2
30	DI	133	ALA	3.1
19	CS	49	ILE	3.1
3	AC	168	TYR	3.1
41	BT	1	MET	3.1
24	DC	220	VAL	3.1
25	DD	60	VAL	3.1
25	DD	126	ASN	3.1
7	CG	59	LEU	3.1
1	CA	1017	U	3.1
38	DQ	59	GLN	3.1
32	DK	74	GLY	3.1
1	CA	1018	G	3.1
22	BA	2125	G	3.1
3	AC	37	PHE	3.1
19	CS	7	LYS	3.1
42	DU	47	LYS	3.1
53	B5	141	PRO	3.1
8	CH	130	ALA	3.1
26	DE	128	ALA	3.1
28	DG	150	ALA	3.1
2	CB	148	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
42	DU	42	VAL	3.1
53	B5	176	VAL	3.1
1	CA	1019	A	3.1
22	BA	1088	A	3.1
22	DA	1597	A	3.1
40	DS	73	LYS	3.1
7	AG	5	ARG	3.1
19	CS	66	MET	3.1
22	BA	1093	G	3.1
46	DY	21	LEU	3.1
26	DE	96	VAL	3.1
29	DH	142	VAL	3.1
30	BI	78	VAL	3.1
22	DA	2150	C	3.1
22	BA	1913	A	3.1
22	BA	2183	A	3.1
27	DF	84	PRO	3.1
7	CG	39	ALA	3.1
14	CN	2	ALA	3.1
41	DT	61	LEU	3.1
7	CG	32	VAL	3.1
29	BH	134	VAL	3.1
33	DL	116	VAL	3.1
22	BA	2124	G	3.1
22	BA	2127	G	3.1
22	BA	2186	G	3.1
40	DS	99	ARG	3.1
19	AS	30	PRO	3.1
22	BA	2117	A	3.1
29	BH	49	ALA	3.1
29	BH	103	VAL	3.0
47	DZ	56	LYS	3.0
33	DL	64	PHE	3.0
50	D2	13	ASN	3.0
22	DA	1248	G	3.0
41	DT	60	THR	3.0
51	D3	49	MET	3.0
26	DE	93	SER	3.0
22	BA	2106	U	3.0
22	DA	1094	U	3.0
41	DT	43	ILE	3.0
27	DF	75	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
38	DQ	21	ALA	3.0
42	DU	2	ALA	3.0
5	AE	11	LEU	3.0
35	DN	38	LEU	3.0
14	CN	11	VAL	3.0
30	BI	70	VAL	3.0
46	DY	46	VAL	3.0
50	D2	33	ARG	3.0
41	DT	75	GLY	3.0
53	B5	193	PHE	3.0
52	D4	23	ILE	3.0
2	CB	161	LEU	3.0
13	CM	69	LEU	3.0
29	BH	113	SER	3.0
30	BI	66	SER	3.0
52	D4	10	LEU	3.0
22	BA	2121	G	3.0
1	AA	1539	C	3.0
22	BA	2153	C	3.0
29	BH	83	LYS	3.0
26	DE	92	HIS	3.0
1	CA	1493	A	3.0
51	D3	14	PHE	3.0
14	CN	30	ILE	3.0
53	B5	208	THR	3.0
10	CJ	71	LEU	3.0
37	DP	97	LEU	3.0
40	DS	97	LEU	3.0
7	CG	128	ALA	3.0
7	CG	150	ALA	3.0
9	CI	44	ALA	3.0
45	DX	77	LYS	3.0
22	BA	2155	U	3.0
27	DF	25	VAL	3.0
30	DI	24	VAL	3.0
41	DT	10	VAL	3.0
22	DA	75	G	3.0
22	DA	268	C	3.0
1	AA	412	A	3.0
22	BA	1057	A	3.0
4	CD	28	ILE	3.0
7	CG	38	THR	3.0

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Mol	Chain	Res	Type	RSRZ
29	BH	58	LEU	3.0
29	DH	6	LEU	3.0
53	B5	189	ASN	3.0
46	DY	61	ALA	3.0
53	B5	143	ALA	3.0
16	AP	20	VAL	3.0
33	DL	80	SER	3.0
22	BA	139	U	2.9
22	BA	2192	U	2.9
25	DD	140	HIS	2.9
53	B5	188	ASP	2.9
24	DC	47	GLY	2.9
4	AD	36	GLN	2.9
22	DA	209	C	2.9
22	DA	2145	C	2.9
3	CC	162	ILE	2.9
29	BH	80	ILE	2.9
30	DI	23	PRO	2.9
1	CA	983	A	2.9
17	CQ	8	LEU	2.9
6	AF	92	THR	2.9
46	DY	44	LYS	2.9
30	DI	115	ALA	2.9
40	DS	40	ASN	2.9
2	AB	14	VAL	2.9
7	CG	27	VAL	2.9
21	AU	47	ARG	2.9
51	D3	26	HIS	2.9
3	CC	37	PHE	2.9
19	CS	10	PHE	2.9
27	BF	113	ASP	2.9
2	AB	13	GLY	2.9
10	CJ	59	LYS	2.9
13	CM	114	LYS	2.9
21	AU	49	LYS	2.9
24	DC	26	LYS	2.9
40	DS	98	LYS	2.9
46	BY	2	LYS	2.9
49	D1	10	LYS	2.9
1	CA	940	C	2.9
22	BA	2160	C	2.9
13	CM	60	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
22	BA	1063	G	2.9
22	DA	277	G	2.9
9	CI	119	ARG	2.9
33	DL	68	SER	2.9
10	AJ	49	PHE	2.9
13	CM	10	PRO	2.9
19	CS	40	ILE	2.9
46	DY	43	LEU	2.9
30	BI	84	ALA	2.9
10	CJ	74	VAL	2.9
29	BH	138	VAL	2.9
32	BK	122	VAL	2.9
23	DB	12	C	2.9
22	DA	477	A	2.9
22	DA	1237	A	2.9
22	BA	549	G	2.9
53	B5	126	SER	2.9
19	CS	5	LEU	2.9
20	CT	67	ILE	2.9
1	CA	4	U	2.9
13	CM	96	PRO	2.9
14	CN	52	PRO	2.9
25	DD	188	LEU	2.9
30	DI	20	PRO	2.9
26	DE	94	GLN	2.9
16	AP	82	ALA	2.9
28	DG	5	ALA	2.9
28	DG	136	ALA	2.9
29	DH	124	THR	2.9
10	CJ	47	GLU	2.9
24	DC	238	ARG	2.9
26	DE	88	ARG	2.9
1	AA	995	C	2.8
22	BA	1098	A	2.8
33	DL	11	GLY	2.8
33	DL	26	GLY	2.8
48	D0	27	SER	2.8
48	D0	39	LEU	2.8
52	D4	18	LYS	2.8
22	BA	1091	G	2.8
53	B5	171	ALA	2.8
53	B5	179	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
28	DG	153	ARG	2.8
32	DK	104	THR	2.8
33	DL	69	ARG	2.8
35	DN	2	ARG	2.8
40	DS	82	MET	2.8
21	CU	44	GLU	2.8
19	CS	69	HIS	2.8
14	AN	42	TRP	2.8
30	BI	87	LYS	2.8
38	DQ	22	LYS	2.8
53	B5	142	LYS	2.8
5	CE	72	ILE	2.8
14	CN	46	LEU	2.8
24	DC	237	GLY	2.8
29	DH	13	GLY	2.8
32	DK	101	GLY	2.8
1	AA	702	A	2.8
1	AA	994	A	2.8
7	CG	41	SER	2.8
14	CN	25	ALA	2.8
26	DE	182	ALA	2.8
53	B5	44	VAL	2.8
30	BI	134	ARG	2.8
30	DI	134	ARG	2.8
22	DA	215	G	2.8
37	DP	102	GLU	2.8
9	CI	127	PHE	2.8
7	CG	137	LYS	2.8
31	DJ	76	HIS	2.8
41	DT	15	HIS	2.8
50	D2	2	LYS	2.8
26	DE	133	LEU	2.8
42	DU	5	ILE	2.8
44	DW	73	GLY	2.8
53	B5	172	ILE	2.8
31	DJ	8	PRO	2.8
1	CA	532	A	2.8
1	CA	1492	A	2.8
4	AD	27	ALA	2.8
13	CM	61	ALA	2.8
22	DA	267	C	2.8
22	DA	795	C	2.8

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Mol	Chain	Res	Type	RSRZ
22	DA	1247	A	2.8
31	DJ	1	MET	2.8
41	DT	41	ALA	2.8
41	DT	46	ALA	2.8
19	CS	3	ARG	2.8
29	BH	78	VAL	2.8
41	DT	12	ARG	2.8
53	B5	146	VAL	2.8
1	AA	1017	U	2.8
22	DA	280	U	2.8
12	AL	25	GLU	2.8
19	CS	74	PHE	2.8
24	DC	7	LYS	2.8
29	DH	83	LYS	2.8
30	BI	69	PHE	2.8
53	B5	38	PHE	2.8
9	CI	54	LEU	2.8
40	BS	63	GLY	2.8
4	AD	38	PRO	2.8
29	BH	93	SER	2.8
13	AM	92	ARG	2.8
19	CS	37	ARG	2.8
26	DE	31	VAL	2.8
29	DH	27	ARG	2.8
29	DH	108	VAL	2.8
22	DA	501	A	2.8
12	CL	44	LYS	2.8
20	AT	5	LYS	2.8
22	DA	2000	C	2.8
42	DU	60	GLU	2.8
53	B5	83	LYS	2.8
24	BC	240	PHE	2.8
53	B5	101	ILE	2.8
25	DD	166	GLY	2.8
30	BI	75	PRO	2.7
9	AI	46	MET	2.7
7	CG	102	ARG	2.7
39	DR	72	VAL	2.7
13	CM	21	SER	2.7
30	BI	88	SER	2.7
29	BH	101	ASP	2.7
9	AI	54	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
13	CM	83	LEU	2.7
22	BA	1058	U	2.7
22	BA	2166	U	2.7
22	DA	1175	A	2.7
48	D0	26	THR	2.7
51	D3	29	LEU	2.7
25	DD	27	ILE	2.7
2	AB	154	MET	2.7
24	DC	239	ASN	2.7
52	D4	36	ARG	2.7
10	CJ	26	VAL	2.7
24	DC	228	VAL	2.7
30	BI	83	ALA	2.7
33	DL	83	ALA	2.7
39	DR	103	ALA	2.7
53	B5	199	ALA	2.7
3	CC	27	LYS	2.7
7	CG	114	LYS	2.7
13	CM	44	LYS	2.7
19	CS	17	LYS	2.7
44	DW	44	LYS	2.7
22	BA	1179	G	2.7
22	DA	214	G	2.7
42	DU	14	LEU	2.7
22	BA	2132	U	2.7
22	BA	2172	U	2.7
22	DA	71	A	2.7
30	DI	32	GLY	2.7
53	B5	52	PRO	2.7
35	DN	1	MET	2.7
22	BA	1914	C	2.7
22	BA	2179	C	2.7
29	BH	66	ASN	2.7
29	BH	145	ASN	2.7
12	CL	124	ALA	2.7
24	DC	245	VAL	2.7
26	DE	39	ALA	2.7
28	DG	43	VAL	2.7
47	DZ	2	ALA	2.7
31	DJ	106	LYS	2.7
10	AJ	90	LEU	2.7
2	CB	67	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
29	BH	143	ILE	2.7
42	DU	15	THR	2.7
45	DX	8	THR	2.7
22	BA	138	U	2.7
22	DA	1311	G	2.7
26	DE	89	PRO	2.7
39	DR	40	MET	2.7
49	D1	18	GLY	2.7
10	CJ	72	ARG	2.7
22	BA	2154	A	2.7
4	CD	151	LYS	2.7
10	CJ	61	ALA	2.7
20	CT	69	LYS	2.7
21	AU	54	LYS	2.7
40	DS	47	VAL	2.7
45	DX	54	LYS	2.7
51	D3	25	LYS	2.7
53	B5	75	VAL	2.7
14	CN	27	LEU	2.7
21	AU	16	LEU	2.7
35	DN	44	LEU	2.7
43	DV	42	LEU	2.7
13	CM	39	ILE	2.7
25	DD	25	THR	2.7
43	DV	43	ASP	2.7
43	DV	82	TYR	2.7
7	CG	34	GLY	2.7
53	B5	91	GLY	2.7
14	CN	61	ARG	2.6
53	B5	28	ARG	2.6
49	B1	53	LYS	2.6
17	CQ	13	VAL	2.6
29	DH	146	VAL	2.6
32	DK	35	VAL	2.6
13	CM	15	ALA	2.6
29	BH	105	ALA	2.6
53	B5	90	ALA	2.6
22	DA	1205	A	2.6
19	CS	47	LEU	2.6
41	DT	7	LEU	2.6
1	AA	990	C	2.6
7	AG	7	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
22	BA	2146	C	2.6
8	CH	2	SER	2.6
13	CM	20	THR	2.6
30	DI	52	GLY	2.6
31	DJ	74	TYR	2.6
41	BT	90	GLY	2.6
53	B5	96	GLY	2.6
46	DY	29	ARG	2.6
21	CU	54	LYS	2.6
24	DC	242	LYS	2.6
36	DO	3	LYS	2.6
42	DU	33	LYS	2.6
9	CI	111	VAL	2.6
4	CD	36	GLN	2.6
33	DL	92	LEU	2.6
5	CE	70	ASN	2.6
26	DE	77	ILE	2.6
29	BH	139	PHE	2.6
22	DA	1245	G	2.6
22	DA	2642	G	2.6
1	AA	1536	C	2.6
22	DA	1330	C	2.6
2	AB	130	THR	2.6
21	AU	51	SER	2.6
29	DH	79	THR	2.6
30	DI	128	SER	2.6
53	B5	122	GLY	2.6
12	AL	15	LYS	2.6
17	CQ	11	ARG	2.6
38	DQ	13	ARG	2.6
40	DS	92	ARG	2.6
41	DT	66	LYS	2.6
49	D1	42	VAL	2.6
1	AA	991	U	2.6
22	DA	1217	U	2.6
22	DA	2796	U	2.6
29	DH	100	ALA	2.6
30	DI	77	ALA	2.6
36	DO	57	ALA	2.6
46	DY	56	LEU	2.6
35	DN	18	GLN	2.6
26	DE	108	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
48	D0	6	ASN	2.6
50	D2	26	ASN	2.6
1	CA	1016	A	2.6
42	DU	37	GLU	2.6
14	AN	52	PRO	2.6
24	DC	29	PRO	2.6
9	CI	124	ARG	2.6
10	CJ	48	ARG	2.6
35	DN	40	LYS	2.6
53	B5	61	GLY	2.6
22	DA	974	G	2.6
22	DA	1171	G	2.6
1	CA	1320	C	2.6
19	CS	12	ASP	2.6
8	CH	63	LEU	2.6
13	CM	19	LEU	2.6
29	DH	90	LEU	2.6
36	DO	23	ALA	2.6
40	DS	46	LEU	2.6
49	D1	11	LEU	2.6
10	CJ	40	ILE	2.6
20	CT	13	GLN	2.6
22	BA	2131	U	2.6
22	BA	2149	U	2.6
22	DA	2585	U	2.6
26	DE	158	PHE	2.6
2	AB	131	LYS	2.6
29	BH	60	GLU	2.6
29	BH	68	ARG	2.6
30	BI	26	PRO	2.6
19	CS	8	GLY	2.6
53	B5	97	GLY	2.6
1	AA	1019	A	2.6
22	BA	2171	A	2.6
9	AI	6	TYR	2.6
19	CS	63	THR	2.6
30	DI	46	THR	2.6
10	CJ	94	ALA	2.5
29	BH	54	LEU	2.6
43	DV	22	ALA	2.5
22	DA	880	G	2.5
22	DA	1404	C	2.5

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Mol	Chain	Res	Type	RSRZ
30	DI	69	PHE	2.5
41	DT	74	ILE	2.5
29	DH	18	GLN	2.5
22	BA	546	U	2.5
13	CM	103	LYS	2.5
39	DR	76	LYS	2.5
7	CG	88	PRO	2.5
13	CM	12	HIS	2.5
13	CM	112	PRO	2.5
19	CS	73	GLU	2.5
24	DC	8	PRO	2.5
33	DL	2	ARG	2.5
39	DR	80	ARG	2.5
45	BX	72	ARG	2.5
53	B5	130	ARG	2.5
7	CG	141	VAL	2.5
30	DI	139	VAL	2.5
1	AA	1016	A	2.5
1	CA	1534	A	2.5
22	DA	1808	A	2.5
53	B5	210	LEU	2.5
35	DN	55	ALA	2.5
27	DF	137	ILE	2.5
30	BI	109	ILE	2.5
42	DU	35	ILE	2.5
51	D3	22	PHE	2.5
30	BI	12	GLN	2.5
22	BA	2177	C	2.5
22	BA	2120	G	2.5
22	DA	1068	G	2.5
24	DC	255	LYS	2.5
24	DC	256	LYS	2.5
41	DT	88	LYS	2.5
10	CJ	37	ARG	2.5
10	CJ	38	GLY	2.5
51	D3	28	ASN	2.5
13	CM	16	VAL	2.5
14	AN	34	VAL	2.5
14	AN	45	VAL	2.5
27	DF	74	VAL	2.5
41	BT	93	LEU	2.5
53	B5	65	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
14	CN	20	TYR	2.5
7	AG	150	ALA	2.5
26	DE	86	ALA	2.5
27	DF	55	ALA	2.5
31	DJ	117	ALA	2.5
53	B5	196	ALA	2.5
19	CS	64	ASP	2.5
22	DA	1938	A	2.5
26	BE	7	ASP	2.5
6	CF	93	LYS	2.5
14	CN	7	LYS	2.5
26	DE	115	GLN	2.5
33	DL	14	LYS	2.5
53	B5	201	LYS	2.5
22	BA	846	U	2.5
1	AA	1001	C	2.5
22	DA	143	C	2.5
22	DA	336	C	2.5
29	BH	95	GLY	2.5
30	BI	91	GLY	2.5
30	DI	119	GLY	2.5
42	DU	53	ASN	2.5
1	AA	79	G	2.5
2	CB	163	VAL	2.5
13	CM	64	VAL	2.5
44	BW	10	THR	2.5
48	D0	9	THR	2.5
14	AN	22	ALA	2.5
14	AN	44	ALA	2.5
18	CR	51	TYR	2.5
29	BH	65	ALA	2.5
13	CM	77	ILE	2.5
14	AN	30	ILE	2.5
30	DI	49	ILE	2.5
13	CM	110	LYS	2.5
38	DQ	5	LYS	2.5
38	DQ	44	GLN	2.5
1	AA	977	A	2.5
24	DC	213	TRP	2.5
31	DJ	13	ARG	2.5
40	DS	95	ARG	2.5
41	DT	69	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
7	CG	71	PRO	2.5
29	BH	128	HIS	2.5
22	BA	1066	U	2.5
22	BA	2111	U	2.5
22	BA	2167	U	2.5
22	DA	1061	U	2.5
33	DL	53	GLY	2.5
41	DT	42	GLU	2.5
13	CM	80	LEU	2.5
7	CG	91	VAL	2.5
19	CS	67	VAL	2.5
29	DH	144	VAL	2.5
1	CA	1325	C	2.5
22	DA	1092	C	2.5
22	DA	2146	C	2.5
3	CC	77	ILE	2.5
7	CG	65	ALA	2.5
14	CN	8	ALA	2.5
19	CS	79	THR	2.5
30	BI	115	ALA	2.5
30	DI	84	ALA	2.5
33	DL	72	ALA	2.5
40	DS	85	ILE	2.5
41	DT	22	THR	2.5
42	DU	72	ILE	2.5
42	DU	85	PHE	2.5
1	CA	1024	G	2.4
5	CE	156	LYS	2.4
22	BA	2162	G	2.4
22	DA	205	G	2.4
22	DA	308	G	2.4
28	DG	85	LYS	2.4
29	BH	112	LYS	2.4
31	DJ	111	LYS	2.4
29	DH	82	SER	2.4
13	CM	100	GLN	2.4
53	B5	66	PRO	2.4
53	B5	134	PRO	2.4
1	AA	1493	A	2.4
22	DA	278	A	2.4
28	DG	45	HIS	2.4
12	CL	24	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
16	AP	77	GLU	2.4
2	AB	209	ALA	2.4
30	BI	76	ALA	2.4
47	DZ	32	ILE	2.4
5	AE	31	PHE	2.4
26	DE	130	LYS	2.4
28	DG	177	LYS	2.4
30	BI	71	THR	2.4
29	DH	97	ARG	2.4
45	DX	18	ARG	2.4
4	CD	152	GLN	2.4
26	DE	41	GLN	2.4
30	DI	105	GLN	2.4
10	AJ	91	ASP	2.4
30	DI	26	PRO	2.4
35	DN	109	PRO	2.4
45	DX	31	PRO	2.4
53	B5	93	ASP	2.4
1	AA	988	G	2.4
1	CA	82	G	2.4
1	CA	211	G	2.4
1	CA	212	G	2.4
22	DA	664	G	2.4
22	DA	669	G	2.4
22	DA	1238	G	2.4
7	CG	23	LEU	2.4
33	DL	114	GLY	2.4
41	DT	70	HIS	2.4
26	DE	186	VAL	2.4
29	BH	61	VAL	2.4
1	AA	1021	A	2.4
22	DA	345	A	2.4
22	DA	505	A	2.4
22	DA	1057	A	2.4
22	BA	2181	U	2.4
51	D3	32	ILE	2.4
4	AD	2	ALA	2.4
13	CM	106	ALA	2.4
19	CS	43	ASN	2.4
30	BI	15	ALA	2.4
42	DU	91	LYS	2.4
33	DL	66	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
30	DI	71	THR	2.4
47	DZ	10	THR	2.4
13	CM	87	ARG	2.4
45	DX	28	ARG	2.4
45	DX	50	ARG	2.4
1	CA	83	C	2.4
30	DI	12	GLN	2.4
14	CN	58	SER	2.4
10	CJ	73	LEU	2.4
28	DG	107	LEU	2.4
42	DU	52	LEU	2.4
8	AH	3	MET	2.4
11	AK	43	GLY	2.4
18	CR	74	HIS	2.4
25	DD	78	GLY	2.4
31	DJ	112	GLY	2.4
41	DT	54	GLU	2.4
41	DT	62	VAL	2.4
53	B5	20	VAL	2.4
53	B5	42	VAL	2.4
9	AI	79	ILE	2.4
22	DA	1063	G	2.4
22	DA	2112	G	2.4
22	BA	1060	U	2.4
22	BA	1069	A	2.4
25	DD	127	PHE	2.4
26	DE	183	PHE	2.4
33	DL	118	THR	2.4
13	CM	93	ARG	2.4
13	CM	113	ARG	2.4
33	DL	18	ARG	2.4
52	D4	12	ARG	2.4
53	B5	94	TYR	2.4
30	BI	74	PRO	2.4
51	D3	46	PRO	2.4
2	CB	212	LEU	2.4
7	CG	22	LEU	2.4
50	D2	22	MET	2.4
22	DA	678	C	2.4
22	DA	1072	C	2.4
33	DL	12	SER	2.4
38	DQ	7	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
11	CK	129	VAL	2.4
29	DH	147	VAL	2.4
26	DE	98	LYS	2.4
29	BH	48	GLU	2.4
2	CB	83	ALA	2.4
21	CU	37	PHE	2.4
29	DH	111	ALA	2.4
45	DX	38	PHE	2.4
1	CA	209	U	2.4
1	CA	1050	G	2.4
7	AG	4	ARG	2.4
19	AS	33	THR	2.4
22	DA	99	U	2.4
29	BH	116	ARG	2.4
30	DI	126	THR	2.4
48	D0	23	THR	2.4
50	D2	35	ARG	2.4
22	DA	74	A	2.4
22	DA	213	A	2.4
22	DA	793	A	2.4
22	DA	1322	A	2.4
7	CG	50	LEU	2.3
13	CM	34	LEU	2.3
31	DJ	79	GLY	2.3
9	AI	128	SER	2.3
9	CI	104	VAL	2.3
11	AK	14	LYS	2.3
28	BG	166	ASP	2.3
38	DQ	4	VAL	2.3
48	D0	57	LYS	2.3
53	B5	150	ILE	2.3
22	BA	2150	C	2.3
2	AB	90	PHE	2.3
7	CG	5	ARG	2.3
19	CS	55	ARG	2.3
47	DZ	31	ARG	2.3
53	B5	155	ARG	2.3
36	DO	24	THR	2.3
49	D1	24	THR	2.3
1	AA	88	U	2.3
1	CA	121	U	2.3
1	CA	1321	U	2.3

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Mol	Chain	Res	Type	RSRZ
22	DA	2690	U	2.3
7	CG	2	PRO	2.3
53	B5	69	LEU	2.3
22	BA	2886	A	2.3
22	DA	73	A	2.3
22	DA	203	A	2.3
22	DA	320	A	2.3
22	DA	354	A	2.3
1	AA	1041	G	2.3
22	DA	7	G	2.3
22	DA	51	G	2.3
22	DA	2069	G	2.3
24	DC	27	GLY	2.3
32	DK	66	LYS	2.3
30	BI	61	VAL	2.3
40	DS	76	VAL	2.3
53	B5	63	VAL	2.3
13	CM	7	ILE	2.3
15	AO	2	SER	2.3
17	CQ	26	GLU	2.3
20	AT	6	SER	2.3
42	DU	98	SER	2.3
30	BI	133	ALA	2.3
50	D2	5	PHE	2.3
34	BM	59	ARG	2.3
51	D3	42	ARG	2.3
22	DA	335	C	2.3
22	DA	378	C	2.3
22	DA	1049	C	2.3
29	BH	77	THR	2.3
30	BI	118	THR	2.3
11	AK	119	ASN	2.3
51	D3	57	LEU	2.3
22	DA	499	U	2.3
22	DA	2797	U	2.3
30	BI	22	PRO	2.3
9	CI	32	GLN	2.3
17	CQ	16	LYS	2.3
22	BA	1090	A	2.3
39	DR	75	VAL	2.3
53	B5	68	GLY	2.3
53	B5	207	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
10	CJ	100	ILE	2.3
1	CA	1297	G	2.3
1	CA	1300	G	2.3
7	CG	26	PHE	2.3
22	BA	2115	G	2.3
42	DU	62	GLU	2.3
19	CS	35	SER	2.3
30	BI	41	ALA	2.3
30	BI	110	ALA	2.3
53	B5	212	SER	2.3
31	DJ	120	ARG	2.3
35	DN	46	ARG	2.3
48	D0	52	ARG	2.3
36	DO	48	LEU	2.3
22	BA	2129	C	2.3
22	DA	393	C	2.3
24	DC	265	LYS	2.3
29	DH	41	LYS	2.3
30	DI	72	LYS	2.3
44	DW	76	ASN	2.3
9	CI	7	TYR	2.3
22	DA	2491	U	2.3
24	DC	251	GLN	2.3
7	CG	69	VAL	2.3
9	CI	116	VAL	2.3
25	DD	135	GLY	2.3
27	DF	13	VAL	2.3
2	CB	16	PHE	2.3
22	DA	2406	A	2.3
29	BH	47	PHE	2.3
30	DI	67	PHE	2.3
2	CB	12	ALA	2.3
29	DH	39	ALA	2.3
34	DM	115	GLU	2.3
16	AP	14	ARG	2.3
39	BR	103	ALA	2.3
20	CT	6	SER	2.3
51	D3	54	ASP	2.3
22	DA	60	G	2.3
22	DA	291	G	2.3
22	DA	1236	G	2.3
2	AB	11	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
2	CB	130	THR	2.3
3	CC	44	THR	2.3
10	CJ	79	PRO	2.3
14	CN	98	LYS	2.3
25	DD	197	THR	2.3
26	DE	150	THR	2.3
27	DF	64	LYS	2.3
39	DR	97	LYS	2.3
1	CA	1533	C	2.2
3	CC	78	GLY	2.2
12	CL	92	GLY	2.2
20	CT	36	TYR	2.2
14	CN	71	HIS	2.2
17	CQ	5	ILE	2.2
22	BA	1102	C	2.2
30	BI	16	GLY	2.2
30	BI	31	GLN	2.2
22	BA	2139	U	2.2
22	DA	290	U	2.2
22	DA	355	U	2.2
30	BI	49	ILE	2.2
39	DR	82	HIS	2.2
7	CG	151	PHE	2.2
13	CM	79	ARG	2.2
24	BC	238	ARG	2.2
29	DH	102	ALA	2.2
31	DJ	95	ARG	2.2
53	B5	27	ALA	2.2
1	CA	977	A	2.2
22	BA	613	A	2.2
22	BA	1089	A	2.2
4	CD	23	SER	2.2
33	DL	81	ASP	2.2
46	DY	18	LEU	2.2
34	DM	11	LYS	2.2
40	DS	6	LYS	2.2
41	DT	40	LYS	2.2
54	D6	4	PRO	2.2
27	DF	35	THR	2.2
27	DF	157	THR	2.2
1	CA	1020	G	2.2
22	DA	180	G	2.2

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Mol	Chain	Res	Type	RSRZ
28	DG	20	ASN	2.2
28	DG	23	VAL	2.2
30	DI	8	TYR	2.2
30	DI	30	GLN	2.2
30	DI	35	ILE	2.2
10	CJ	49	PHE	2.2
25	DD	59	ARG	2.2
45	DX	11	ARG	2.2
53	B5	209	PHE	2.2
22	DA	672	C	2.2
21	AU	39	GLU	2.2
21	CU	8	GLU	2.2
29	BH	64	ALA	2.2
53	B5	36	ALA	2.2
46	DY	30	MET	2.2
14	AN	27	LEU	2.2
30	BI	106	LEU	2.2
30	BI	97	LYS	2.2
30	DI	92	LYS	2.2
30	DI	113	LYS	2.2
44	DW	72	LYS	2.2
1	AA	1042	A	2.2
1	CA	1332	A	2.2
22	DA	415	A	2.2
22	DA	1392	A	2.2
42	DU	50	PRO	2.2
49	D1	22	THR	2.2
53	B5	41	THR	2.2
13	AM	7	ILE	2.2
2	CB	149	GLY	2.2
24	BC	237	GLY	2.2
28	DG	21	GLY	2.2
29	BH	107	GLY	2.2
29	DH	120	GLY	2.2
30	BI	13	VAL	2.2
32	DK	29	HIS	2.2
33	DL	65	GLY	2.2
47	DZ	34	HIS	2.2
20	CT	3	ASN	2.2
42	DU	27	ASN	2.2
9	AI	45	ARG	2.2
25	DD	118	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	AA	993	G	2.2
1	CA	987	G	2.2
1	CA	1222	G	2.2
1	CA	1330	U	2.2
4	CD	37	ALA	2.2
9	CI	121	ALA	2.2
14	CN	6	MET	2.2
22	DA	50	U	2.2
22	DA	500	G	2.2
28	DG	174	ALA	2.2
28	DG	33	LEU	2.2
41	DT	11	LEU	2.2
7	CG	149	LYS	2.2
9	CI	68	LYS	2.2
22	DA	228	C	2.2
31	DJ	85	LYS	2.2
35	DN	35	LYS	2.2
37	DP	6	LYS	2.2
42	DU	97	LYS	2.2
52	D4	8	LYS	2.2
53	B5	80	LYS	2.2
10	AJ	75	ASP	2.2
40	DS	94	ASP	2.2
19	CS	77	THR	2.2
22	BA	1073	A	2.2
22	DA	311	A	2.2
26	DE	148	ILE	2.2
26	DE	178	VAL	2.2
28	DG	80	THR	2.2
41	DT	58	VAL	2.2
30	BI	89	GLY	2.2
9	AI	75	GLN	2.2
42	DU	45	HIS	2.2
42	DU	46	GLN	2.2
7	CG	68	ASN	2.2
10	AJ	5	ARG	2.2
29	DH	139	PHE	2.2
30	BI	136	MET	2.2
13	CM	40	ALA	2.2
37	DP	95	ALA	2.2
41	DT	20	ALA	2.2
53	B5	46	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
5	AE	65	GLU	2.2
6	CF	75	GLU	2.2
10	AJ	78	GLU	2.2
25	DD	8	LYS	2.2
26	DE	95	LYS	2.2
26	DE	132	LYS	2.2
29	BH	5	LEU	2.2
29	DH	62	LEU	2.2
35	DN	51	LEU	2.2
40	DS	23	LEU	2.2
22	DA	2151	U	2.2
1	CA	108	G	2.2
1	CA	1220	G	2.2
19	CS	30	PRO	2.2
22	BA	141	G	2.2
22	DA	136	G	2.2
22	DA	266	G	2.2
22	DA	1136	G	2.2
1	CA	1317	C	2.2
14	CN	54	ASP	2.2
22	DA	281	C	2.2
16	CP	2	VAL	2.2
17	CQ	10	GLY	2.1
26	DE	71	GLY	2.1
29	BH	13	GLY	2.1
42	DU	38	GLY	2.1
13	CM	14	HIS	2.1
53	B5	200	HIS	2.1
21	AU	35	ARG	2.1
22	BA	2163	A	2.1
22	DA	2173	A	2.1
41	BT	3	ARG	2.1
7	CG	61	ALA	2.1
7	CG	76	LYS	2.1
14	CN	29	ALA	2.1
14	CN	99	ALA	2.1
26	DE	135	ALA	2.1
26	DE	200	LEU	2.1
30	DI	97	LYS	2.1
41	DT	8	LEU	2.1
36	DO	46	GLU	2.1
1	CA	219	U	2.1

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Mol	Chain	Res	Type	RSRZ
22	DA	931	U	2.1
25	DD	23	PRO	2.1
52	D4	31	PRO	2.1
53	B5	182	PRO	2.1
27	DF	156	ILE	2.1
25	DD	9	VAL	2.1
7	CG	54	SER	2.1
26	DE	82	GLY	2.1
1	AA	841	C	2.1
1	CA	1304	G	2.1
13	CM	101	ARG	2.1
22	BA	2161	C	2.1
22	BA	2308	G	2.1
22	DA	68	G	2.1
22	DA	237	C	2.1
22	DA	376	G	2.1
22	DA	410	G	2.1
22	DA	1235	G	2.1
22	DA	1382	G	2.1
22	DA	2072	C	2.1
22	DA	2755	C	2.1
24	DC	48	ARG	2.1
34	DM	129	THR	2.1
38	DQ	3	ARG	2.1
40	DS	7	HIS	2.1
14	CN	97	LYS	2.1
12	CL	23	ALA	2.1
16	CP	17	TYR	2.1
36	DO	68	LYS	2.1
25	DD	192	ALA	2.1
25	DD	209	ALA	2.1
26	DE	3	LEU	2.1
53	B5	186	LEU	2.1
22	DA	911	A	2.1
22	DA	2602	A	2.1
30	BI	37	GLU	2.1
13	CM	85	CYS	2.1
28	DG	8	PRO	2.1
41	DT	80	TRP	2.1
1	CA	632	U	2.1
1	CA	1240	U	2.1
1	CA	1286	U	2.1

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Mol	Chain	Res	Type	RSRZ
1	CA	1537	U	2.1
22	BA	1065	U	2.1
22	DA	12	U	2.1
22	DA	224	U	2.1
7	AG	27	VAL	2.1
26	DE	83	VAL	2.1
27	DF	40	VAL	2.1
30	BI	98	VAL	2.1
15	CO	17	ARG	2.1
27	DF	80	ARG	2.1
28	DG	166	ASP	2.1
30	DI	117	MET	2.1
29	BH	132	PHE	2.1
30	BI	48	SER	2.1
45	DX	20	HIS	2.1
50	D2	45	SER	2.1
12	AL	123	LYS	2.1
19	CS	70	LYS	2.1
30	BI	40	LYS	2.1
51	D3	39	LYS	2.1
1	CA	1028	C	2.1
21	AU	50	ALA	2.1
21	CU	50	ALA	2.1
22	DA	41	C	2.1
22	DA	130	C	2.1
22	DA	509	C	2.1
22	DA	2313	C	2.1
23	DB	60	C	2.1
25	DD	132	ALA	2.1
38	DQ	12	ALA	2.1
51	D3	60	ALA	2.1
1	CA	973	G	2.1
1	CA	993	G	2.1
1	CA	1255	G	2.1
22	DA	682	G	2.1
22	DA	1310	G	2.1
22	DA	1343	G	2.1
22	DA	1702	G	2.1
22	DA	2319	G	2.1
23	BB	41	G	2.1
53	B5	25	GLU	2.1
22	BA	142	A	2.1

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Mol	Chain	Res	Type	RSRZ
22	BA	2170	A	2.1
28	DG	26	ILE	2.1
33	DL	101	ILE	2.1
39	DR	49	ILE	2.1
1	CA	1025	U	2.1
22	DA	288	U	2.1
22	DA	589	U	2.1
4	AD	25	VAL	2.1
5	CE	74	VAL	2.1
9	CI	19	VAL	2.1
13	CM	25	VAL	2.1
28	DG	11	VAL	2.1
3	CC	155	GLY	2.1
4	AD	63	ARG	2.1
19	AS	55	ARG	2.1
25	DD	169	ARG	2.1
27	DF	82	GLY	2.1
30	DI	99	GLY	2.1
34	DM	16	ARG	2.1
44	DW	11	ARG	2.1
45	DX	55	GLY	2.1
53	B5	211	ARG	2.1
7	AG	142	HIS	2.1
9	AI	129	LYS	2.1
17	AQ	16	LYS	2.1
2	CB	10	LEU	2.1
6	CF	39	LEU	2.1
7	CG	30	LEU	2.1
9	CI	98	LEU	2.1
10	CJ	52	LEU	2.1
33	DL	42	SER	2.1
42	DU	31	SER	2.1
14	AN	2	ALA	2.1
1	CA	1038	C	2.1
1	CA	1218	C	2.1
10	CJ	66	GLU	2.1
18	AR	20	GLU	2.1
22	DA	105	C	2.1
22	DA	444	C	2.1
22	DA	679	C	2.1
22	DA	2422	C	2.1
30	DI	130	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
53	B5	86	GLU	2.1
32	DK	89	ASN	2.1
29	DH	32	PRO	2.1
30	BI	129	ILE	2.1
1	AA	1014	A	2.1
1	AA	1167	A	2.1
22	BA	1068	G	2.1
22	DA	327	G	2.1
22	DA	1090	A	2.1
22	DA	1721	G	2.1
22	DA	2156	G	2.1
22	DA	2410	G	2.1
23	DB	41	G	2.1
39	DR	92	TRP	2.1
30	BI	5	VAL	2.1
42	DU	36	VAL	2.1
1	CA	1183	U	2.1
10	CJ	5	ARG	2.1
12	CL	14	ARG	2.1
21	AU	17	ARG	2.1
22	DA	1599	U	2.1
24	DC	5	LYS	2.1
27	DF	76	GLY	2.1
48	D0	7	LYS	2.1
50	D2	17	GLY	2.1
2	CB	32	PHE	2.1
36	DO	97	PHE	2.1
44	DW	79	PHE	2.1
9	CI	63	LEU	2.0
13	CM	95	LEU	2.0
33	DL	82	LEU	2.0
2	CB	88	ASP	2.0
10	CJ	60	ASP	2.0
30	BI	132	THR	2.0
6	CF	100	SER	2.0
13	CM	5	ALA	2.0
13	CM	30	SER	2.0
16	AP	22	ALA	2.0
30	DI	114	ALA	2.0
31	DJ	6	ALA	2.0
46	DY	33	ALA	2.0
35	DN	112	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
12	AL	5	ASN	2.0
13	CM	4	ILE	2.0
19	AS	9	PRO	2.0
29	DH	118	PRO	2.0
42	DU	69	ASN	2.0
1	CA	1322	C	2.0
22	DA	337	C	2.0
22	DA	343	C	2.0
22	DA	1251	C	2.0
6	AF	91	ARG	2.0
13	AM	3	ARG	2.0
19	AS	3	ARG	2.0
27	DF	149	VAL	2.0
31	DJ	116	ARG	2.0
38	DQ	31	VAL	2.0
40	DS	20	VAL	2.0
41	BT	69	ARG	2.0
53	B5	74	ARG	2.0
28	DG	27	LYS	2.0
52	D4	9	LYS	2.0
1	CA	1216	A	2.0
1	CA	1441	A	2.0
5	AE	102	GLY	2.0
11	CK	43	GLY	2.0
22	DA	502	A	2.0
30	DI	25	GLY	2.0
32	DK	112	PHE	2.0
53	B5	204	GLY	2.0
5	AE	115	LEU	2.0
22	BA	1083	U	2.0
22	BA	2109	U	2.0
22	DA	1065	U	2.0
22	DA	1325	U	2.0
46	BY	6	LEU	2.0
1	AA	1003	G	2.0
1	CA	220	G	2.0
22	BA	2110	G	2.0
22	DA	289	G	2.0
22	DA	1087	G	2.0
39	DR	19	THR	2.0
14	CN	44	ALA	2.0
26	DE	50	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
29	BH	39	ALA	2.0
30	DI	18	ALA	2.0
30	DI	111	GLN	2.0
40	DS	44	ALA	2.0
41	DT	45	ALA	2.0
53	B5	92	ALA	2.0
53	B5	167	ASP	2.0
4	CD	153	SER	2.0
17	CQ	20	SER	2.0
29	BH	136	SER	2.0
53	B5	180	SER	2.0
5	CE	30	ILE	2.0
10	AJ	81	GLU	2.0
30	DI	62	TYR	2.0
51	D3	64	TYR	2.0
24	DC	49	ILE	2.0
42	DU	103	ILE	2.0
2	CB	74	ARG	2.0
19	CS	58	VAL	2.0
27	DF	69	LYS	2.0
28	DG	17	VAL	2.0
28	DG	158	LYS	2.0
29	DH	134	VAL	2.0
41	DT	63	VAL	2.0
44	DW	75	LYS	2.0
53	B5	206	LYS	2.0
9	AI	20	PHE	2.0
9	AI	39	PHE	2.0
24	DC	33	LEU	2.0
25	DD	156	PHE	2.0
27	DF	39	GLY	2.0
28	DG	52	PHE	2.0
34	DM	119	LEU	2.0
51	D3	21	GLY	2.0
22	DA	1064	C	2.0
22	DA	1172	C	2.0
22	DA	1289	C	2.0
29	DH	135	HIS	2.0

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

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	MHU	D6	5	15/16	0.83	0.20	45,56,65,65	0
54	04X	D6	6	15/16	0.83	0.15	46,56,70,73	0
54	004	D6	7	10/11	0.86	0.12	40,51,56,56	0
54	DBB	D6	3	6/7	0.89	0.20	45,52,56,63	0
54	MHW	D6	1	9/10	0.90	0.12	36,47,54,54	0
54	04X	B6	6	15/16	0.95	0.09	1,3,15,15	0
54	004	B6	7	10/11	0.96	0.09	0,0,1,2	0
54	MHU	B6	5	15/16	0.96	0.09	0,1,3,6	0
54	DBB	B6	3	6/7	0.97	0.08	0,1,1,4	0
54	MHW	B6	1	9/10	0.97	0.06	0,1,2,9	0

5.3 Carbohydrates ⓘ

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
55	MG	DA	3027	1/1	-0.34	0.47	96,96,96,96	0
55	MG	BA	3137	1/1	0.13	0.53	66,66,66,66	0
55	MG	DA	3134	1/1	0.15	0.37	100,100,100,100	0
55	MG	DA	3127	1/1	0.25	0.15	86,86,86,86	0
55	MG	BA	3016	1/1	0.48	0.34	59,59,59,59	0
55	MG	DA	3114	1/1	0.48	0.15	80,80,80,80	0
55	MG	CA	1649	1/1	0.59	0.33	71,71,71,71	0
55	MG	DA	3103	1/1	0.60	0.16	83,83,83,83	0
55	MG	DA	3042	1/1	0.60	0.22	68,68,68,68	0
55	MG	BA	3062	1/1	0.65	0.32	57,57,57,57	0
55	MG	DA	3101	1/1	0.65	0.21	78,78,78,78	0
55	MG	DA	3132	1/1	0.66	0.26	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	CA	1630	1/1	0.66	0.17	105,105,105,105	0
55	MG	DA	3154	1/1	0.66	0.33	70,70,70,70	0
55	MG	DA	3116	1/1	0.67	0.17	96,96,96,96	0
55	MG	DA	3041	1/1	0.70	0.14	92,92,92,92	0
55	MG	DA	3113	1/1	0.70	0.35	77,77,77,77	0
55	MG	DA	3063	1/1	0.71	0.24	93,93,93,93	0
55	MG	DA	3062	1/1	0.73	0.59	104,104,104,104	0
55	MG	AA	1668	1/1	0.74	0.21	58,58,58,58	0
55	MG	DA	3120	1/1	0.74	0.24	97,97,97,97	0
55	MG	DA	3057	1/1	0.75	0.22	88,88,88,88	0
55	MG	AA	1658	1/1	0.76	0.18	72,72,72,72	0
55	MG	DA	3110	1/1	0.76	0.18	48,48,48,48	0
55	MG	DA	3094	1/1	0.77	0.12	93,93,93,93	0
55	MG	DA	3033	1/1	0.78	0.17	71,71,71,71	0
55	MG	DA	3014	1/1	0.78	0.15	80,80,80,80	0
55	MG	DA	3028	1/1	0.78	0.11	83,83,83,83	0
55	MG	BA	3099	1/1	0.79	0.22	64,64,64,64	0
55	MG	DA	3121	1/1	0.79	0.21	78,78,78,78	0
55	MG	DA	3061	1/1	0.80	0.21	80,80,80,80	0
55	MG	BA	3041	1/1	0.80	0.33	2,2,2,2	0
55	MG	CA	1636	1/1	0.80	0.15	113,113,113,113	0
55	MG	DA	3074	1/1	0.80	0.17	68,68,68,68	0
55	MG	DA	3093	1/1	0.80	0.20	101,101,101,101	0
55	MG	DA	3138	1/1	0.80	0.25	52,52,52,52	0
55	MG	DA	3020	1/1	0.80	0.15	83,83,83,83	0
55	MG	CA	1635	1/1	0.81	0.10	120,120,120,120	0
55	MG	DA	3036	1/1	0.81	0.11	70,70,70,70	0
55	MG	DA	3007	1/1	0.81	0.13	101,101,101,101	0
55	MG	CA	1646	1/1	0.81	0.21	65,65,65,65	0
55	MG	DA	3045	1/1	0.81	0.14	95,95,95,95	0
55	MG	AA	1665	1/1	0.82	0.09	48,48,48,48	0
55	MG	DA	3136	1/1	0.82	0.17	84,84,84,84	0
55	MG	BA	3058	1/1	0.82	0.32	45,45,45,45	0
55	MG	DA	3149	1/1	0.82	0.22	54,54,54,54	0
55	MG	CA	1656	1/1	0.82	0.15	53,53,53,53	0
55	MG	DA	3100	1/1	0.83	0.18	81,81,81,81	0
55	MG	CA	1643	1/1	0.83	0.28	56,56,56,56	0
55	MG	CA	1633	1/1	0.83	0.16	78,78,78,78	0
55	MG	CA	1641	1/1	0.83	0.24	67,67,67,67	0
55	MG	DA	3163	1/1	0.83	0.07	71,71,71,71	0
55	MG	DA	3166	1/1	0.83	0.20	57,57,57,57	0
55	MG	AA	1659	1/1	0.84	0.10	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	AA	1660	1/1	0.84	0.38	70,70,70,70	0
55	MG	DA	3148	1/1	0.84	0.15	58,58,58,58	0
55	MG	DA	3108	1/1	0.84	0.11	72,72,72,72	0
55	MG	DA	3150	1/1	0.84	0.21	61,61,61,61	0
55	MG	AA	1649	1/1	0.84	0.09	46,46,46,46	0
55	MG	DA	3095	1/1	0.84	0.09	80,80,80,80	0
55	MG	BA	3134	1/1	0.84	0.28	47,47,47,47	0
55	MG	DA	3139	1/1	0.85	0.26	49,49,49,49	0
55	MG	DA	3146	1/1	0.85	0.15	84,84,84,84	0
55	MG	BA	3048	1/1	0.85	0.12	53,53,53,53	0
55	MG	CA	1645	1/1	0.85	0.12	40,40,40,40	0
55	MG	BA	3084	1/1	0.85	0.19	49,49,49,49	0
55	MG	CA	1625	1/1	0.85	0.10	43,43,43,43	0
55	MG	DA	3072	1/1	0.85	0.12	80,80,80,80	0
55	MG	BA	3037	1/1	0.85	0.22	35,35,35,35	0
55	MG	BA	3088	1/1	0.86	0.21	37,37,37,37	0
55	MG	DA	3025	1/1	0.86	0.21	56,56,56,56	0
55	MG	DA	3009	1/1	0.86	0.19	81,81,81,81	0
55	MG	DA	3157	1/1	0.86	0.27	63,63,63,63	0
55	MG	DA	3076	1/1	0.86	0.12	70,70,70,70	0
55	MG	CA	1628	1/1	0.86	0.14	98,98,98,98	0
55	MG	BA	3083	1/1	0.87	0.15	20,20,20,20	0
55	MG	CA	1647	1/1	0.87	0.08	45,45,45,45	0
55	MG	CA	1605	1/1	0.87	0.10	88,88,88,88	0
55	MG	DA	3147	1/1	0.87	0.09	60,60,60,60	0
55	MG	DA	3073	1/1	0.87	0.16	72,72,72,72	0
55	MG	DA	3124	1/1	0.87	0.09	51,51,51,51	0
55	MG	DA	3125	1/1	0.87	0.13	92,92,92,92	0
55	MG	DA	3049	1/1	0.87	0.09	109,109,109,109	0
55	MG	DA	3016	1/1	0.87	0.21	78,78,78,78	0
55	MG	DA	3079	1/1	0.87	0.10	92,92,92,92	0
55	MG	CA	1638	1/1	0.87	0.09	84,84,84,84	0
55	MG	DA	3145	1/1	0.88	0.18	67,67,67,67	0
55	MG	BA	3081	1/1	0.88	0.08	16,16,16,16	0
55	MG	DA	3109	1/1	0.88	0.13	50,50,50,50	0
55	MG	BA	3147	1/1	0.88	0.20	39,39,39,39	0
55	MG	BA	3159	1/1	0.88	0.14	21,21,21,21	0
55	MG	BA	3173	1/1	0.88	0.10	32,32,32,32	0
55	MG	DA	3153	1/1	0.88	0.25	62,62,62,62	0
55	MG	BA	3193	1/1	0.88	0.13	42,42,42,42	0
55	MG	AA	1655	1/1	0.88	0.24	45,45,45,45	0
55	MG	AA	1670	1/1	0.88	0.14	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	DA	3144	1/1	0.88	0.15	30,30,30,30	0
55	MG	CA	1614	1/1	0.89	0.08	49,49,49,49	0
55	MG	AA	1653	1/1	0.89	0.24	51,51,51,51	0
55	MG	BA	3056	1/1	0.89	0.13	29,29,29,29	0
55	MG	DA	3047	1/1	0.89	0.09	80,80,80,80	0
55	MG	DA	3005	1/1	0.89	0.18	94,94,94,94	0
55	MG	BA	3191	1/1	0.89	0.23	20,20,20,20	0
55	MG	DA	3030	1/1	0.89	0.14	72,72,72,72	0
55	MG	AA	1647	1/1	0.89	0.15	58,58,58,58	0
55	MG	DA	3117	1/1	0.89	0.19	73,73,73,73	0
55	MG	DA	3141	1/1	0.89	0.22	41,41,41,41	0
55	MG	BA	3003	1/1	0.89	0.09	23,23,23,23	0
55	MG	DA	3126	1/1	0.90	0.09	59,59,59,59	0
55	MG	AA	1644	1/1	0.90	0.17	58,58,58,58	0
55	MG	DA	3058	1/1	0.90	0.13	73,73,73,73	0
55	MG	BA	3136	1/1	0.90	0.13	34,34,34,34	0
55	MG	AA	1662	1/1	0.90	0.11	47,47,47,47	0
55	MG	AA	1645	1/1	0.90	0.08	53,53,53,53	0
55	MG	CA	1655	1/1	0.90	0.15	51,51,51,51	0
55	MG	CA	1642	1/1	0.90	0.26	29,29,29,29	0
55	MG	DA	3161	1/1	0.90	0.13	49,49,49,49	0
55	MG	DA	3003	1/1	0.90	0.19	92,92,92,92	0
55	MG	BA	3154	1/1	0.90	0.12	34,34,34,34	0
55	MG	DA	3082	1/1	0.91	0.08	66,66,66,66	0
55	MG	DA	3143	1/1	0.91	0.12	39,39,39,39	0
55	MG	AA	1635	1/1	0.91	0.13	65,65,65,65	0
55	MG	AA	1652	1/1	0.91	0.35	56,56,56,56	0
55	MG	DA	3059	1/1	0.91	0.21	70,70,70,70	0
55	MG	BA	3174	1/1	0.91	0.07	27,27,27,27	0
55	MG	CA	1631	1/1	0.91	0.10	92,92,92,92	0
55	MG	BA	3089	1/1	0.91	0.11	22,22,22,22	0
55	MG	DA	3107	1/1	0.91	0.08	48,48,48,48	0
55	MG	DA	3011	1/1	0.91	0.11	60,60,60,60	0
55	MG	AA	1632	1/1	0.91	0.09	54,54,54,54	0
55	MG	BA	3148	1/1	0.91	0.09	24,24,24,24	0
55	MG	DA	3158	1/1	0.91	0.16	49,49,49,49	0
55	MG	CA	1654	1/1	0.91	0.06	58,58,58,58	0
55	MG	BA	3132	1/1	0.91	0.21	50,50,50,50	0
55	MG	DA	3165	1/1	0.91	0.09	68,68,68,68	0
55	MG	DA	3140	1/1	0.91	0.17	28,28,28,28	0
55	MG	BA	3060	1/1	0.92	0.12	9,9,9,9	0
55	MG	CA	1652	1/1	0.92	0.07	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	DA	3050	1/1	0.92	0.10	83,83,83,83	0
55	MG	DA	3089	1/1	0.92	0.06	78,78,78,78	0
55	MG	DA	3092	1/1	0.92	0.07	77,77,77,77	0
55	MG	DA	3055	1/1	0.92	0.12	41,41,41,41	0
55	MG	BA	3047	1/1	0.92	0.07	9,9,9,9	0
55	MG	BA	3079	1/1	0.92	0.06	37,37,37,37	0
55	MG	BA	3149	1/1	0.92	0.14	27,27,27,27	0
55	MG	CA	1615	1/1	0.92	0.11	55,55,55,55	0
55	MG	DA	3156	1/1	0.92	0.18	42,42,42,42	0
55	MG	BA	3102	1/1	0.92	0.08	10,10,10,10	0
55	MG	AA	1672	1/1	0.92	0.28	49,49,49,49	0
55	MG	DA	3070	1/1	0.92	0.15	86,86,86,86	0
55	MG	CA	1629	1/1	0.92	0.07	80,80,80,80	0
55	MG	AA	1666	1/1	0.92	0.21	41,41,41,41	0
55	MG	BA	3005	1/1	0.92	0.09	42,42,42,42	0
55	MG	DA	3167	1/1	0.92	0.27	43,43,43,43	0
55	MG	AA	1650	1/1	0.93	0.08	37,37,37,37	0
55	MG	BA	3015	1/1	0.93	0.08	6,6,6,6	0
55	MG	CA	1601	1/1	0.93	0.07	45,45,45,45	0
55	MG	DA	3133	1/1	0.93	0.19	53,53,53,53	0
55	MG	AA	1663	1/1	0.93	0.07	41,41,41,41	0
55	MG	DA	3087	1/1	0.93	0.07	69,69,69,69	0
55	MG	CA	1606	1/1	0.93	0.09	70,70,70,70	0
55	MG	DA	3090	1/1	0.93	0.09	80,80,80,80	0
55	MG	BA	3026	1/1	0.93	0.15	36,36,36,36	0
55	MG	CA	1651	1/1	0.93	0.07	50,50,50,50	0
55	MG	BA	3061	1/1	0.93	0.20	28,28,28,28	0
55	MG	DA	3043	1/1	0.93	0.09	82,82,82,82	0
55	MG	CA	1617	1/1	0.93	0.08	40,40,40,40	0
55	MG	BA	3151	1/1	0.93	0.14	49,49,49,49	0
55	MG	BA	3153	1/1	0.93	0.13	11,11,11,11	0
55	MG	DA	3104	1/1	0.93	0.13	67,67,67,67	0
55	MG	AA	1609	1/1	0.93	0.07	35,35,35,35	0
55	MG	BA	3157	1/1	0.93	0.20	27,27,27,27	0
55	MG	DA	3151	1/1	0.93	0.31	49,49,49,49	0
55	MG	DA	3006	1/1	0.93	0.06	98,98,98,98	0
55	MG	BA	3158	1/1	0.93	0.10	15,15,15,15	0
55	MG	DA	3008	1/1	0.93	0.16	100,100,100,100	0
55	MG	BA	3103	1/1	0.93	0.16	13,13,13,13	0
55	MG	BA	3002	1/1	0.93	0.09	15,15,15,15	0
55	MG	DA	3159	1/1	0.93	0.17	61,61,61,61	0
55	MG	AA	1657	1/1	0.93	0.10	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BA	3187	1/1	0.93	0.12	25,25,25,25	0
55	MG	DA	3071	1/1	0.93	0.05	96,96,96,96	0
55	MG	DA	3017	1/1	0.93	0.09	84,84,84,84	0
55	MG	BA	3190	1/1	0.93	0.17	39,39,39,39	0
56	VIF	DA	3001	38/38	0.93	0.13	34,47,57,61	0
55	MG	BA	3035	1/1	0.94	0.19	47,47,47,47	0
55	MG	AA	1654	1/1	0.94	0.14	30,30,30,30	0
55	MG	DA	3065	1/1	0.94	0.11	43,43,43,43	0
55	MG	DA	3142	1/1	0.94	0.20	40,40,40,40	0
55	MG	DA	3029	1/1	0.94	0.11	65,65,65,65	0
55	MG	BA	3072	1/1	0.94	0.12	23,23,23,23	0
55	MG	AA	1614	1/1	0.94	0.16	55,55,55,55	0
55	MG	AA	1661	1/1	0.94	0.11	53,53,53,53	0
55	MG	DA	3111	1/1	0.94	0.07	43,43,43,43	0
55	MG	DA	3112	1/1	0.94	0.08	70,70,70,70	0
55	MG	AA	1669	1/1	0.94	0.14	51,51,51,51	0
55	MG	AA	1616	1/1	0.94	0.07	50,50,50,50	0
55	MG	BA	3138	1/1	0.94	0.20	4,4,4,4	0
55	MG	DA	3080	1/1	0.94	0.05	101,101,101,101	0
55	MG	BA	3184	1/1	0.94	0.09	10,10,10,10	0
55	MG	DA	3155	1/1	0.94	0.14	45,45,45,45	0
55	MG	DA	3012	1/1	0.94	0.17	74,74,74,74	0
55	MG	CA	1648	1/1	0.94	0.18	30,30,30,30	0
55	MG	AA	1630	1/1	0.94	0.14	63,63,63,63	0
55	MG	BA	3189	1/1	0.94	0.11	44,44,44,44	0
55	MG	DA	3160	1/1	0.94	0.10	74,74,74,74	0
55	MG	DA	3019	1/1	0.94	0.09	85,85,85,85	0
55	MG	BA	3028	1/1	0.94	0.15	15,15,15,15	0
55	MG	BA	3091	1/1	0.94	0.04	23,23,23,23	0
55	MG	DA	3098	1/1	0.94	0.10	73,73,73,73	0
55	MG	DA	3099	1/1	0.94	0.10	50,50,50,50	0
55	MG	DA	3168	1/1	0.94	0.11	47,47,47,47	0
55	MG	D2	101	1/1	0.94	0.08	77,77,77,77	0
55	MG	DA	3026	1/1	0.94	0.12	67,67,67,67	0
55	MG	AA	1627	1/1	0.95	0.11	58,58,58,58	0
55	MG	BA	3020	1/1	0.95	0.07	8,8,8,8	0
55	MG	AA	1651	1/1	0.95	0.20	40,40,40,40	0
55	MG	DA	3128	1/1	0.95	0.07	71,71,71,71	0
55	MG	DA	3078	1/1	0.95	0.11	83,83,83,83	0
55	MG	CA	1644	1/1	0.95	0.06	55,55,55,55	0
55	MG	BA	3150	1/1	0.95	0.14	45,45,45,45	0
55	MG	DA	3081	1/1	0.95	0.10	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	DA	3137	1/1	0.95	0.11	88,88,88,88	0
55	MG	BA	3074	1/1	0.95	0.06	14,14,14,14	0
55	MG	DA	3084	1/1	0.95	0.12	72,72,72,72	0
55	MG	DA	3085	1/1	0.95	0.06	78,78,78,78	0
55	MG	BA	3075	1/1	0.95	0.11	29,29,29,29	0
55	MG	BA	3112	1/1	0.95	0.07	8,8,8,8	0
55	MG	CA	1608	1/1	0.95	0.10	63,63,63,63	0
55	MG	CA	1650	1/1	0.95	0.16	44,44,44,44	0
55	MG	CA	1611	1/1	0.95	0.13	82,82,82,82	0
55	MG	BA	3113	1/1	0.95	0.05	13,13,13,13	0
55	MG	BA	3125	1/1	0.95	0.17	20,20,20,20	0
55	MG	BA	3049	1/1	0.95	0.09	13,13,13,13	0
55	MG	DA	3046	1/1	0.95	0.05	77,77,77,77	0
55	MG	CA	1622	1/1	0.95	0.10	51,51,51,51	0
55	MG	DA	3002	1/1	0.95	0.06	65,65,65,65	0
55	MG	BA	3166	1/1	0.95	0.17	36,36,36,36	0
55	MG	DA	3052	1/1	0.95	0.05	49,49,49,49	0
55	MG	DA	3053	1/1	0.95	0.06	45,45,45,45	0
55	MG	DA	3054	1/1	0.95	0.07	41,41,41,41	0
55	MG	CA	1627	1/1	0.95	0.14	76,76,76,76	0
55	MG	BA	3055	1/1	0.95	0.08	6,6,6,6	0
55	MG	AA	1612	1/1	0.95	0.06	37,37,37,37	0
55	MG	BA	3175	1/1	0.95	0.13	33,33,33,33	0
55	MG	BA	3177	1/1	0.95	0.17	29,29,29,29	0
55	MG	DA	3162	1/1	0.95	0.08	35,35,35,35	0
55	MG	DA	3010	1/1	0.95	0.05	68,68,68,68	0
55	MG	DA	3164	1/1	0.95	0.17	57,57,57,57	0
55	MG	DA	3115	1/1	0.95	0.05	51,51,51,51	0
55	MG	BA	3178	1/1	0.95	0.10	13,13,13,13	0
55	MG	AA	1656	1/1	0.95	0.10	36,36,36,36	0
55	MG	BA	3185	1/1	0.95	0.23	25,25,25,25	0
55	MG	CA	1637	1/1	0.95	0.12	64,64,64,64	0
55	MG	AA	1671	1/1	0.95	0.39	47,47,47,47	0
55	MG	BA	3122	1/1	0.96	0.09	39,39,39,39	0
55	MG	DA	3056	1/1	0.96	0.09	66,66,66,66	0
55	MG	CA	1613	1/1	0.96	0.05	24,24,24,24	0
55	MG	AA	1619	1/1	0.96	0.16	37,37,37,37	0
55	MG	BA	3165	1/1	0.96	0.10	5,5,5,5	0
55	MG	AA	1631	1/1	0.96	0.12	48,48,48,48	0
55	MG	CA	1619	1/1	0.96	0.06	40,40,40,40	0
55	MG	CA	1621	1/1	0.96	0.07	71,71,71,71	0
55	MG	DA	3064	1/1	0.96	0.08	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BA	3170	1/1	0.96	0.06	33,33,33,33	0
55	MG	DA	3066	1/1	0.96	0.06	39,39,39,39	0
55	MG	BA	3171	1/1	0.96	0.07	24,24,24,24	0
55	MG	AA	1626	1/1	0.96	0.06	19,19,19,19	0
55	MG	AA	1634	1/1	0.96	0.05	42,42,42,42	0
55	MG	AA	1664	1/1	0.96	0.07	42,42,42,42	0
55	MG	BA	3176	1/1	0.96	0.09	13,13,13,13	0
55	MG	DA	3075	1/1	0.96	0.07	63,63,63,63	0
55	MG	AA	1617	1/1	0.96	0.08	51,51,51,51	0
55	MG	DA	3077	1/1	0.96	0.07	65,65,65,65	0
55	MG	BA	3141	1/1	0.96	0.14	26,26,26,26	0
55	MG	BA	3180	1/1	0.96	0.22	40,40,40,40	0
55	MG	BA	3182	1/1	0.96	0.09	20,20,20,20	0
55	MG	BA	3183	1/1	0.96	0.14	24,24,24,24	0
55	MG	BA	3142	1/1	0.96	0.24	5,5,5,5	0
55	MG	CA	1639	1/1	0.96	0.05	49,49,49,49	0
55	MG	BA	3145	1/1	0.96	0.09	41,41,41,41	0
55	MG	DA	3086	1/1	0.96	0.09	72,72,72,72	0
55	MG	BA	3186	1/1	0.96	0.08	32,32,32,32	0
55	MG	DA	3032	1/1	0.96	0.05	63,63,63,63	0
55	MG	BA	3146	1/1	0.96	0.11	15,15,15,15	0
55	MG	DA	3091	1/1	0.96	0.09	76,76,76,76	0
55	MG	DA	3034	1/1	0.96	0.06	62,62,62,62	0
55	MG	BA	3100	1/1	0.96	0.07	14,14,14,14	0
55	MG	DA	3038	1/1	0.96	0.05	75,75,75,75	0
55	MG	DA	3040	1/1	0.96	0.07	60,60,60,60	0
55	MG	AA	1637	1/1	0.96	0.05	16,16,16,16	0
55	MG	BA	3006	1/1	0.96	0.06	51,51,51,51	0
55	MG	BA	3192	1/1	0.96	0.08	34,34,34,34	0
55	MG	BA	3105	1/1	0.96	0.13	0,0,0,0	0
55	MG	AA	1667	1/1	0.96	0.11	54,54,54,54	0
55	MG	CA	1604	1/1	0.96	0.05	89,89,89,89	0
55	MG	DA	3105	1/1	0.96	0.06	67,67,67,67	0
55	MG	DA	3106	1/1	0.96	0.12	72,72,72,72	0
55	MG	DA	3048	1/1	0.96	0.09	53,53,53,53	0
55	MG	AA	1638	1/1	0.96	0.05	77,77,77,77	0
55	MG	BA	3115	1/1	0.96	0.06	17,17,17,17	0
55	MG	CA	1653	1/1	0.96	0.11	42,42,42,42	0
55	MG	DB	203	1/1	0.96	0.05	83,83,83,83	0
55	MG	BA	3116	1/1	0.96	0.15	50,50,50,50	0
55	MG	CA	1609	1/1	0.96	0.07	77,77,77,77	0
55	MG	BA	3024	1/1	0.97	0.06	4,4,4,4	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	AA	1643	1/1	0.97	0.15	25,25,25,25	0
55	MG	CA	1624	1/1	0.97	0.05	47,47,47,47	0
55	MG	BA	3077	1/1	0.97	0.12	61,61,61,61	0
55	MG	BA	3181	1/1	0.97	0.11	19,19,19,19	0
55	MG	DA	3119	1/1	0.97	0.08	46,46,46,46	0
55	MG	BA	3078	1/1	0.97	0.04	31,31,31,31	0
55	MG	DA	3015	1/1	0.97	0.06	44,44,44,44	0
55	MG	BA	3111	1/1	0.97	0.07	24,24,24,24	0
55	MG	DA	3068	1/1	0.97	0.04	47,47,47,47	0
55	MG	DA	3069	1/1	0.97	0.05	60,60,60,60	0
55	MG	AA	1624	1/1	0.97	0.05	35,35,35,35	0
55	MG	BA	3080	1/1	0.97	0.07	17,17,17,17	0
55	MG	DA	3129	1/1	0.97	0.09	75,75,75,75	0
55	MG	CA	1632	1/1	0.97	0.08	74,74,74,74	0
55	MG	DA	3021	1/1	0.97	0.04	64,64,64,64	0
55	MG	DA	3022	1/1	0.97	0.07	62,62,62,62	0
55	MG	DA	3135	1/1	0.97	0.07	53,53,53,53	0
55	MG	DA	3023	1/1	0.97	0.09	42,42,42,42	0
55	MG	AA	1603	1/1	0.97	0.14	48,48,48,48	0
55	MG	AA	1610	1/1	0.97	0.11	63,63,63,63	0
55	MG	BA	3117	1/1	0.97	0.06	3,3,3,3	0
55	MG	BA	3119	1/1	0.97	0.05	14,14,14,14	0
55	MG	BA	3120	1/1	0.97	0.19	32,32,32,32	0
55	MG	BA	3121	1/1	0.97	0.06	7,7,7,7	0
55	MG	DA	3031	1/1	0.97	0.06	57,57,57,57	0
55	MG	AA	1636	1/1	0.97	0.08	42,42,42,42	0
55	MG	BA	3194	1/1	0.97	0.08	32,32,32,32	0
55	MG	BB	204	1/1	0.97	0.26	21,21,21,21	0
55	MG	DA	3035	1/1	0.97	0.04	41,41,41,41	0
55	MG	BD	301	1/1	0.97	0.07	27,27,27,27	0
55	MG	DA	3037	1/1	0.97	0.04	54,54,54,54	0
55	MG	BA	3160	1/1	0.97	0.07	29,29,29,29	0
55	MG	DA	3039	1/1	0.97	0.08	63,63,63,63	0
55	MG	CA	1602	1/1	0.97	0.10	69,69,69,69	0
55	MG	BA	3085	1/1	0.97	0.14	16,16,16,16	0
55	MG	BA	3086	1/1	0.97	0.05	5,5,5,5	0
55	MG	DA	3096	1/1	0.97	0.07	75,75,75,75	0
55	MG	BA	3167	1/1	0.97	0.04	21,21,21,21	0
55	MG	CA	1607	1/1	0.97	0.07	47,47,47,47	0
55	MG	BA	3169	1/1	0.97	0.12	34,34,34,34	0
55	MG	BA	3133	1/1	0.97	0.10	37,37,37,37	0
55	MG	DA	3102	1/1	0.97	0.05	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	CA	1610	1/1	0.97	0.07	64,64,64,64	0
55	MG	AA	1605	1/1	0.97	0.06	33,33,33,33	0
55	MG	CA	1612	1/1	0.97	0.05	44,44,44,44	0
55	MG	DA	3051	1/1	0.97	0.05	54,54,54,54	0
55	MG	BA	3172	1/1	0.97	0.05	32,32,32,32	0
55	MG	BA	3063	1/1	0.97	0.04	6,6,6,6	0
55	MG	BA	3070	1/1	0.97	0.07	50,50,50,50	0
55	MG	DB	201	1/1	0.97	0.05	97,97,97,97	0
55	MG	AA	1613	1/1	0.97	0.04	30,30,30,30	0
55	MG	CA	1618	1/1	0.97	0.05	45,45,45,45	0
56	VIF	BA	3001	38/38	0.97	0.07	0,2,7,10	0
55	MG	BA	3140	1/1	0.97	0.12	3,3,3,3	0
55	MG	DA	3004	1/1	0.98	0.04	65,65,65,65	0
55	MG	BA	3032	1/1	0.98	0.09	5,5,5,5	0
55	MG	BA	3162	1/1	0.98	0.16	37,37,37,37	0
55	MG	BA	3163	1/1	0.98	0.09	31,31,31,31	0
55	MG	DA	3118	1/1	0.98	0.05	66,66,66,66	0
55	MG	BA	3164	1/1	0.98	0.21	19,19,19,19	0
55	MG	AA	1608	1/1	0.98	0.04	16,16,16,16	0
55	MG	AA	1601	1/1	0.98	0.03	41,41,41,41	0
55	MG	BA	3040	1/1	0.98	0.04	3,3,3,3	0
55	MG	BA	3168	1/1	0.98	0.09	35,35,35,35	0
55	MG	CA	1616	1/1	0.98	0.03	33,33,33,33	0
55	MG	AA	1628	1/1	0.98	0.04	35,35,35,35	0
55	MG	BA	3044	1/1	0.98	0.07	19,19,19,19	0
55	MG	BA	3045	1/1	0.98	0.04	21,21,21,21	0
55	MG	DA	3018	1/1	0.98	0.05	51,51,51,51	0
55	MG	CA	1620	1/1	0.98	0.04	65,65,65,65	0
55	MG	BA	3124	1/1	0.98	0.07	5,5,5,5	0
55	MG	BA	3004	1/1	0.98	0.04	25,25,25,25	0
55	MG	CA	1623	1/1	0.98	0.09	35,35,35,35	0
55	MG	BA	3126	1/1	0.98	0.05	4,4,4,4	0
55	MG	AA	1639	1/1	0.98	0.05	60,60,60,60	0
55	MG	CA	1626	1/1	0.98	0.05	43,43,43,43	0
55	MG	AA	1640	1/1	0.98	0.04	45,45,45,45	0
55	MG	BA	3052	1/1	0.98	0.04	3,3,3,3	0
55	MG	DA	3083	1/1	0.98	0.04	49,49,49,49	0
55	MG	BA	3053	1/1	0.98	0.04	6,6,6,6	0
55	MG	BA	3179	1/1	0.98	0.10	34,34,34,34	0
55	MG	BA	3013	1/1	0.98	0.05	0,0,0,0	0
55	MG	AA	1602	1/1	0.98	0.11	46,46,46,46	0
55	MG	DA	3088	1/1	0.98	0.03	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BA	3139	1/1	0.98	0.18	0,0,0,0	0
55	MG	BA	3092	1/1	0.98	0.04	55,55,55,55	0
55	MG	BA	3094	1/1	0.98	0.04	30,30,30,30	0
55	MG	BA	3095	1/1	0.98	0.04	20,20,20,20	0
55	MG	DA	3152	1/1	0.98	0.10	47,47,47,47	0
55	MG	BA	3143	1/1	0.98	0.20	14,14,14,14	0
55	MG	BA	3096	1/1	0.98	0.10	10,10,10,10	0
55	MG	BA	3188	1/1	0.98	0.05	16,16,16,16	0
55	MG	AA	1606	1/1	0.98	0.04	41,41,41,41	0
55	MG	DA	3097	1/1	0.98	0.05	51,51,51,51	0
55	MG	AA	1621	1/1	0.98	0.04	35,35,35,35	0
55	MG	AA	1646	1/1	0.98	0.14	55,55,55,55	0
55	MG	BA	3025	1/1	0.98	0.02	0,0,0,0	0
55	MG	BA	3104	1/1	0.98	0.04	18,18,18,18	0
55	MG	AA	1607	1/1	0.98	0.04	41,41,41,41	0
55	MG	BB	203	1/1	0.98	0.04	15,15,15,15	0
55	MG	BA	3152	1/1	0.98	0.04	18,18,18,18	0
55	MG	BA	3108	1/1	0.98	0.05	9,9,9,9	0
55	MG	BQ	201	1/1	0.98	0.10	1,1,1,1	0
55	MG	BA	3110	1/1	0.98	0.12	0,0,0,0	0
55	MG	BA	3155	1/1	0.98	0.04	26,26,26,26	0
55	MG	CA	1603	1/1	0.98	0.04	36,36,36,36	0
55	MG	DB	202	1/1	0.98	0.05	65,65,65,65	0
55	MG	BA	3156	1/1	0.98	0.10	23,23,23,23	0
55	MG	BA	3069	1/1	0.98	0.05	0,0,0,0	0
55	MG	AA	1625	1/1	0.98	0.04	33,33,33,33	0
55	MG	BA	3030	1/1	0.98	0.10	12,12,12,12	0
55	MG	BA	3093	1/1	0.99	0.06	38,38,38,38	0
55	MG	BA	3050	1/1	0.99	0.04	6,6,6,6	0
55	MG	BA	3051	1/1	0.99	0.03	5,5,5,5	0
55	MG	AA	1615	1/1	0.99	0.05	50,50,50,50	0
55	MG	BA	3098	1/1	0.99	0.03	2,2,2,2	0
55	MG	DA	3060	1/1	0.99	0.04	43,43,43,43	0
55	MG	BA	3021	1/1	0.99	0.06	2,2,2,2	0
55	MG	BA	3054	1/1	0.99	0.05	2,2,2,2	0
55	MG	BA	3022	1/1	0.99	0.03	0,0,0,0	0
55	MG	DA	3122	1/1	0.99	0.03	44,44,44,44	0
55	MG	BA	3023	1/1	0.99	0.05	0,0,0,0	0
55	MG	BA	3057	1/1	0.99	0.05	3,3,3,3	0
55	MG	AA	1622	1/1	0.99	0.10	17,17,17,17	0
55	MG	DA	3067	1/1	0.99	0.03	42,42,42,42	0
55	MG	BA	3106	1/1	0.99	0.14	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BA	3161	1/1	0.99	0.03	13,13,13,13	0
55	MG	DA	3130	1/1	0.99	0.07	39,39,39,39	0
55	MG	DA	3131	1/1	0.99	0.03	67,67,67,67	0
55	MG	AA	1633	1/1	0.99	0.03	41,41,41,41	0
55	MG	DA	3013	1/1	0.99	0.04	34,34,34,34	0
55	MG	BA	3109	1/1	0.99	0.10	1,1,1,1	0
55	MG	AA	1648	1/1	0.99	0.03	57,57,57,57	0
55	MG	BA	3027	1/1	0.99	0.04	4,4,4,4	0
55	MG	AA	1604	1/1	0.99	0.02	58,58,58,58	0
55	MG	BA	3064	1/1	0.99	0.08	0,0,0,0	0
55	MG	BA	3114	1/1	0.99	0.07	0,0,0,0	0
55	MG	BA	3065	1/1	0.99	0.10	0,0,0,0	0
55	MG	BA	3067	1/1	0.99	0.06	1,1,1,1	0
55	MG	BA	3068	1/1	0.99	0.07	0,0,0,0	0
55	MG	BA	3118	1/1	0.99	0.03	1,1,1,1	0
55	MG	DA	3024	1/1	0.99	0.03	61,61,61,61	0
55	MG	BA	3029	1/1	0.99	0.03	2,2,2,2	0
55	MG	AA	1641	1/1	0.99	0.05	15,15,15,15	0
55	MG	BA	3071	1/1	0.99	0.04	5,5,5,5	0
55	MG	BA	3007	1/1	0.99	0.02	17,17,17,17	0
55	MG	BA	3123	1/1	0.99	0.06	0,0,0,0	0
55	MG	BA	3034	1/1	0.99	0.16	0,0,0,0	0
55	MG	BA	3008	1/1	0.99	0.04	22,22,22,22	0
55	MG	BA	3076	1/1	0.99	0.04	4,4,4,4	0
55	MG	BA	3127	1/1	0.99	0.07	6,6,6,6	0
55	MG	CA	1634	1/1	0.99	0.03	52,52,52,52	0
55	MG	BA	3129	1/1	0.99	0.04	5,5,5,5	0
55	MG	BA	3036	1/1	0.99	0.03	0,0,0,0	0
55	MG	BA	3009	1/1	0.99	0.02	5,5,5,5	0
55	MG	BA	3038	1/1	0.99	0.10	0,0,0,0	0
55	MG	BA	3135	1/1	0.99	0.04	2,2,2,2	0
55	MG	CA	1640	1/1	0.99	0.04	31,31,31,31	0
55	MG	BA	3039	1/1	0.99	0.02	0,0,0,0	0
55	MG	BA	3011	1/1	0.99	0.06	1,1,1,1	0
55	MG	BA	3012	1/1	0.99	0.03	25,25,25,25	0
55	MG	DA	3044	1/1	0.99	0.06	47,47,47,47	0
55	MG	BA	3043	1/1	0.99	0.04	11,11,11,11	0
55	MG	AA	1642	1/1	0.99	0.04	15,15,15,15	0
55	MG	BA	3014	1/1	0.99	0.04	0,0,0,0	0
55	MG	BA	3087	1/1	0.99	0.09	1,1,1,1	0
55	MG	BA	3046	1/1	0.99	0.03	2,2,2,2	0
55	MG	BB	201	1/1	0.99	0.02	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	AA	1629	1/1	0.99	0.04	54,54,54,54	0
55	MG	BA	3090	1/1	0.99	0.04	1,1,1,1	0
55	MG	AA	1620	1/1	0.99	0.03	59,59,59,59	0
55	MG	BA	3018	1/1	0.99	0.07	0,0,0,0	0
55	MG	BB	202	1/1	1.00	0.02	2,2,2,2	0
55	MG	BA	3101	1/1	1.00	0.02	2,2,2,2	0
55	MG	BA	3010	1/1	1.00	0.02	0,0,0,0	0
55	MG	AA	1611	1/1	1.00	0.01	19,19,19,19	0
55	MG	AA	1618	1/1	1.00	0.01	41,41,41,41	0
55	MG	BA	3017	1/1	1.00	0.07	1,1,1,1	0
55	MG	BA	3066	1/1	1.00	0.04	1,1,1,1	0
55	MG	BA	3107	1/1	1.00	0.12	0,0,0,0	0
55	MG	AA	1623	1/1	1.00	0.04	46,46,46,46	0
55	MG	BA	3144	1/1	1.00	0.11	8,8,8,8	0
55	MG	BA	3031	1/1	1.00	0.04	2,2,2,2	0
55	MG	BA	3019	1/1	1.00	0.05	12,12,12,12	0
55	MG	BA	3082	1/1	1.00	0.04	0,0,0,0	0
55	MG	BA	3128	1/1	1.00	0.01	0,0,0,0	0
55	MG	DA	3123	1/1	1.00	0.07	37,37,37,37	0
55	MG	BA	3059	1/1	1.00	0.06	13,13,13,13	0
55	MG	BA	3130	1/1	1.00	0.02	0,0,0,0	0
55	MG	BA	3131	1/1	1.00	0.06	0,0,0,0	0
55	MG	BA	3097	1/1	1.00	0.04	5,5,5,5	0
55	MG	BA	3033	1/1	1.00	0.03	4,4,4,4	0
55	MG	BA	3042	1/1	1.00	0.05	11,11,11,11	0
55	MG	BA	3073	1/1	1.00	0.04	2,2,2,2	0
57	ZN	B4	101	1/1	1.00	0.02	24,24,24,24	0
57	ZN	D4	101	1/1	1.00	0.02	86,86,86,86	0

5.5 Other polymers ⓘ

There are no such residues in this entry.