



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 28, 2026 – 01:57 PM UTC

PDB ID : 4V7M / pdb_00004v7m
Title : The structures of Capreomycin bound to the 70S ribosome.
Authors : Stanley, R.E.; Blaha, G.
Deposited on : 2009-11-12
Resolution : 3.45 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
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

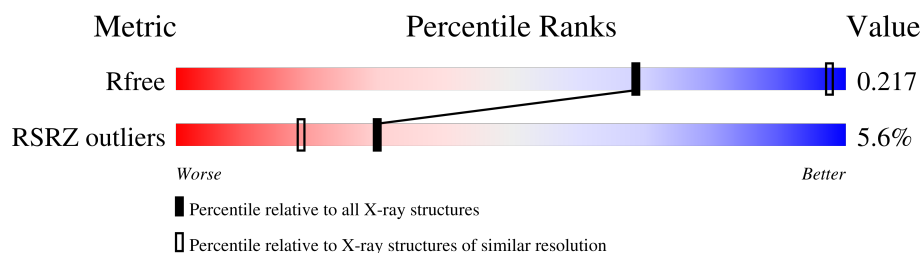
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.45 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1070 (3.50-3.42)
RSRZ outliers	180081	1070 (3.50-3.42)

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
60	MG	AA	1630	-	-	-	X
60	MG	AA	1648	-	-	-	X
60	MG	BA	3201	-	-	-	X

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 293848 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1495	Total	C	N	O	P	0	0	0
			32132	14303	5953	10382	1494			
1	CA	1493	Total	C	N	O	P	0	0	0
			32098	14287	5956	10363	1492			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			
2	CB	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			
3	CC	206	Total	C	N	O	S	0	0	1
			1604	1011	314	278	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			
4	CD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			
5	CE	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
6	CF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
7	CG	154	Total	C	N	O	S	0	0	0
			1249	776	251	217	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
8	CH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AI	127	Total	C	N	O		0	0	0
			1006	637	195	174				
9	CI	127	Total	C	N	O		0	0	0
			1006	637	195	174				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	99	Total	C	N	O	S	0	0	1
			795	499	157	138	1			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	CJ	99	Total	C	N	O	S	0	0	1
			795	499	157	138	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AK	116	Total	C	N	O	S	0	0	0
			864	537	164	160	3			
11	CK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			
12	CL	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	122	Total	C	N	O	S	0	0	1
			965	597	200	166	2			
13	CM	118	Total	C	N	O	S	0	0	0
			937	579	193	163	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
14	CN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- 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
			734	459	147	126	2			
15	CO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			
16	CP	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	100	Total	C	N	O	S	0	0	1
			824	528	152	142	2			
17	CQ	100	Total	C	N	O	S	0	0	1
			824	528	152	142	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AR	70	Total	C	N	O	0	0	0
			574	367	112	95			
18	CR	70	Total	C	N	O	0	0	0
			574	367	112	95			

- 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	1
			630	403	115	110	2			
19	CS	79	Total	C	N	O	S	0	0	1
			630	403	115	110	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			
20	CT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AU	25	Total	C	N	O	0	0	1
			209	128	51	30			
21	CU	25	Total	C	N	O	0	0	1
			209	128	51	30			

- Molecule 22 is a RNA chain called RNA (5'-R(*AP*AP*AP*AP*AP*GP*GP*AP*AP*AP*UP*A*AP*AP*AP*AP*UP*GP*CP*AP*GP*UP*UP*CP*AP*AP*UP*CP*UP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	10	Total	C	N	O	P	0	0	0
			205	93	40	63	9			
22	CV	10	Total	C	N	O	P	0	0	0
			213	97	42	65	9			

- Molecule 23 is a RNA chain called tRNA-Gln.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AW	74	Total	C	N	O	P	0	0	0
			1573	702	279	518	74			
23	CW	74	Total	C	N	O	P	0	0	0
			1573	702	279	518	74			

- Molecule 24 is a RNA chain called tRNA-Met.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AX	77	Total	C	N	O	P	0	0	0
			1639	732	297	534	76			

- Molecule 25 is a RNA chain called tRNA-Gln.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	AY	75	Total	C	N	O	P	0	0	0
			1591	711	280	526	74			
25	CY	75	Total	C	N	O	P	0	0	0
			1591	711	280	526	74			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AY	33	G	C	conflict	GB CP001790.1
AY	44	U	A	conflict	GB CP001790.1
CY	33	G	C	conflict	GB CP001790.1
CY	44	U	A	conflict	GB CP001790.1

- Molecule 26 is a protein called capreomycin IA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
26	AZ	6	Total	C	N	O	0	0	0
			47	25	14	8			
26	CZ	6	Total	C	N	O	0	0	0
			47	25	14	8			

- Molecule 27 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BA	2789	Total	C	N	O	P	0	0	0
			60072	26734	11238	19312	2788			
27	DA	2775	Total	C	N	O	P	0	0	0
			59767	26598	11176	19219	2774			

- Molecule 28 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			
28	DB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			

- Molecule 29 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
29	BC	191	Total	C	N	O	0	0	1
			1142	691	221	230			
29	DC	191	Total	C	N	O	0	0	1
			1142	691	221	230			

- Molecule 30 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BD	272	Total	C	N	O	S	0	0	1
			2105	1329	417	356	3			
30	DD	272	Total	C	N	O	S	0	0	1
			2105	1329	417	356	3			

- Molecule 31 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BE	205	Total	C	N	O	S	0	0	1
			1564	988	300	270	6			
31	DE	205	Total	C	N	O	S	0	0	1
			1564	988	300	270	6			

- Molecule 32 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BF	206	Total	C	N	O	S	0	0	1
			1607	1024	301	280	2			
32	DF	208	Total	C	N	O	S	0	0	1
			1624	1035	304	282	3			

- Molecule 33 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			
33	DG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			

- Molecule 34 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BH	161	Total	C	N	O	S	0	0	0
			1233	783	227	222	1			
34	DH	160	Total	C	N	O	S	0	0	1
			1223	773	229	220	1			

- Molecule 35 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BI	146	Total	C	N	O	S	0	0	1
			1132	723	201	207	1			
35	DI	146	Total	C	N	O	S	0	0	1
			1132	723	201	207	1			

- Molecule 36 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BN	139	Total	C	N	O	S	0	0	1
			1105	712	207	182	4			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	DN	139	Total	C	N	O	S	0	0	1
			1105	712	207	182	4			

- Molecule 37 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			
37	DO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 38 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BP	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			
38	DP	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			

- Molecule 39 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BQ	139	Total	C	N	O	S	0	0	0
			1107	707	209	184	7			
39	DQ	138	Total	C	N	O	S	0	0	0
			1094	697	205	185	7			

- Molecule 40 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	BR	117	Total	C	N	O	0	0	0
			960	599	202	159			
40	DR	117	Total	C	N	O	0	0	0
			960	599	202	159			

- Molecule 41 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
41	BS	99	Total	C	N	O	0	0	1
			771	486	155	130			
41	DS	99	Total	C	N	O	0	0	1
			771	486	155	130			

- Molecule 42 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BT	138	Total	C	N	O	S	0	0	1
			1142	710	235	196	1			
42	DT	138	Total	C	N	O	S	0	0	1
			1142	710	235	196	1			

- Molecule 43 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BU	117	Total	C	N	O	S	0	0	0
			958	604	202	151	1			
43	DU	117	Total	C	N	O	S	0	0	0
			958	604	202	151	1			

- Molecule 44 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
44	DV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 45 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BW	113	Total	C	N	O	S	0	0	0
			896	563	176	155	2			
45	DW	113	Total	C	N	O	S	0	0	0
			896	563	176	155	2			

- Molecule 46 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
46	BX	93	Total	C	N	O	0	0	1
			726	471	132	123			
46	DX	93	Total	C	N	O	0	0	1
			726	471	132	123			

- Molecule 47 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BY	88	Total	C	N	O	S	0	0	1
			672	432	131	105	4			
47	DY	101	Total	C	N	O	S	0	0	1
			776	500	149	123	4			

- Molecule 48 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BZ	177	Total	C	N	O	S	0	0	1
			1404	897	253	252	2			
48	DZ	177	Total	C	N	O	S	0	0	1
			1404	897	253	252	2			

- Molecule 49 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	B0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			
49	D0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B1	94	Total	C	N	O	S	0	0	1
			732	460	146	125	1			
50	D1	94	Total	C	N	O	S	0	0	1
			732	460	146	125	1			

- Molecule 51 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			
51	D2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			

- Molecule 52 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B3	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	D3	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			

- Molecule 53 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B4	49	Total	C	N	O	S	0	0	1
			344	215	60	65	4			
53	D4	49	Total	C	N	O	S	0	0	1
			344	215	60	65	4			

- Molecule 54 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
54	D5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 55 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	B6	48	Total	C	N	O	S	0	0	1
			402	249	83	66	4			
55	D6	46	Total	C	N	O	S	0	0	1
			390	241	80	65	4			

- Molecule 56 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	B7	49	Total	C	N	O	S	0	0	1
			419	257	105	55	2			
56	D7	49	Total	C	N	O	S	0	0	1
			419	257	105	55	2			

- Molecule 57 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	B8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			
57	D8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			

- Molecule 58 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	B9	36	Total	C	N	O	S	0	0	0
			299	183	67	46	3			
58	D9	36	Total	C	N	O	S	0	0	0
			299	183	67	46	3			

- Molecule 59 is a RNA chain called RNA (77-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
59	CX	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CX	46	G	A	conflict	GB CP001637.1

- Molecule 60 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	AA	114	Total	Mg	0	0
			114	114		
60	AG	1	Total	Mg	0	0
			1	1		
60	AW	4	Total	Mg	0	0
			4	4		
60	AX	9	Total	Mg	0	0
			9	9		
60	BA	334	Total	Mg	0	0
			334	334		
60	BB	5	Total	Mg	0	0
			5	5		
60	BD	1	Total	Mg	0	0
			1	1		
60	BE	3	Total	Mg	0	0
			3	3		
60	BF	1	Total	Mg	0	0
			1	1		
60	BG	1	Total	Mg	0	0
			1	1		
60	BP	2	Total	Mg	0	0
			2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	BR	1	Total 1	Mg 1	0	0
60	BU	2	Total 2	Mg 2	0	0
60	BX	1	Total 1	Mg 1	0	0
60	B0	3	Total 3	Mg 3	0	0
60	B5	1	Total 1	Mg 1	0	0
60	CA	102	Total 102	Mg 102	0	0
60	CE	1	Total 1	Mg 1	0	0
60	CK	1	Total 1	Mg 1	0	0
60	CV	1	Total 1	Mg 1	0	0
60	CW	4	Total 4	Mg 4	0	0
60	DA	239	Total 239	Mg 239	0	0
60	DB	3	Total 3	Mg 3	0	0
60	DD	2	Total 2	Mg 2	0	0
60	DE	1	Total 1	Mg 1	0	0
60	DF	1	Total 1	Mg 1	0	0
60	DO	1	Total 1	Mg 1	0	0
60	D0	1	Total 1	Mg 1	0	0
60	D5	1	Total 1	Mg 1	0	0
60	D7	1	Total 1	Mg 1	0	0

- Molecule 61 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	AD	1	Total 1	Zn 1	0	0
61	B4	1	Total 1	Zn 1	0	0
61	B5	1	Total 1	Zn 1	0	0
61	B9	1	Total 1	Zn 1	0	0
61	CD	1	Total 1	Zn 1	0	0
61	D4	1	Total 1	Zn 1	0	0
61	D5	1	Total 1	Zn 1	0	0
61	D9	1	Total 1	Zn 1	0	0

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

3 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.35Å 448.24Å 631.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.45 50.00 – 3.45	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.45) 85.3 (50.00-3.45)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 3.40Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.218 , 0.268 0.218 , 0.217	Depositor DCC
R_{free} test set	33507 reflections (4.13%)	wwPDB-VP
Wilson B-factor (Å ²)	74.9	Xtriage
Anisotropy	0.240	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	293848	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.86% 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	$\# Z > 2$
26	KBE	CZ	1	26	8,8,9	1.33	1 (12%)	6,8,10	2.26	2 (33%)
26	UAL	CZ	3	26	6,8,9	2.67	2 (33%)	4,9,11	1.48	1 (25%)
26	MYN	AZ	4	26	8,11,12	2.47	1 (12%)	6,14,16	1.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	DPP	AZ	2	26	4,5,6	0.54	0	1,5,7	0.55	0
26	DPP	CZ	2	26	4,5,6	0.85	0	1,5,7	0.30	0
26	MYN	CZ	4	26	8,11,12	1.97	1 (12%)	6,14,16	1.67	2 (33%)
26	DPP	CZ	5	26	4,5,6	0.74	0	1,5,7	0.31	0
26	KBE	AZ	1	26	8,8,9	1.61	1 (12%)	6,8,10	2.62	2 (33%)
26	DPP	AZ	5	26	4,5,6	0.50	0	1,5,7	0.25	0
26	UAL	AZ	3	26	6,8,9	2.68	2 (33%)	4,9,11	1.96	1 (25%)

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
26	KBE	CZ	1	26	-	1/7/7/8	-
26	UAL	CZ	3	26	-	0/3/7/9	-
26	MYN	AZ	4	26	-	0/1/16/18	0/1/1/1
26	DPP	AZ	2	26	-	2/2/4/6	-
26	DPP	CZ	2	26	-	1/2/4/6	-
26	MYN	CZ	4	26	-	0/1/16/18	0/1/1/1
26	DPP	CZ	5	26	-	0/2/4/6	-
26	KBE	AZ	1	26	-	1/7/7/8	-
26	DPP	AZ	5	26	-	0/2/4/6	-
26	UAL	AZ	3	26	-	0/3/7/9	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	AZ	4	MYN	CZ-NE	6.81	1.41	1.34
26	CZ	4	MYN	CZ-NE	5.07	1.39	1.34
26	CZ	3	UAL	C-CA	4.76	1.53	1.45
26	AZ	3	UAL	C1-N1	-4.51	1.33	1.40
26	AZ	3	UAL	C-CA	4.47	1.52	1.45
26	CZ	3	UAL	C1-N1	-4.23	1.33	1.40
26	AZ	1	KBE	CA-C	-4.10	1.39	1.50
26	CZ	1	KBE	CA-C	-3.59	1.40	1.50

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	AZ	1	KBE	CB-CA-C	5.71	121.39	112.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	CZ	1	KBE	CB-CA-C	4.86	120.02	112.17
26	AZ	3	UAL	O-C-CA	-3.72	120.72	125.39
26	AZ	1	KBE	O-C-CA	-2.80	117.22	125.38
26	CZ	3	UAL	O-C-CA	-2.73	121.97	125.39
26	CZ	1	KBE	O-C-CA	-2.53	118.01	125.38
26	CZ	4	MYN	CG-CB-CA	-2.53	109.33	112.44
26	CZ	4	MYN	NZ-CZ-NE	2.22	119.73	117.93

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	AZ	1	KBE	C-CA-CB-N
26	CZ	1	KBE	C-CA-CB-N
26	AZ	2	DPP	N-CA-CB-NG
26	AZ	2	DPP	C-CA-CB-NG
26	CZ	2	DPP	N-CA-CB-NG

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 850 ligands modelled in this entry, 850 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

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	1495/1508 (99%)	-0.02	34 (2%) 61 38	32, 72, 154, 200	0
1	CA	1493/1508 (99%)	0.20	58 (3%) 43 25	38, 81, 158, 200	0
2	AB	235/256 (91%)	0.42	14 (5%) 27 17	69, 98, 133, 148	0
2	CB	235/256 (91%)	0.62	15 (6%) 25 17	74, 103, 147, 165	0
3	AC	207/239 (86%)	0.22	6 (2%) 53 32	66, 86, 109, 114	0
3	CC	206/239 (86%)	0.59	13 (6%) 26 17	76, 98, 123, 136	0
4	AD	208/209 (99%)	0.22	10 (4%) 35 21	52, 73, 87, 92	0
4	CD	208/209 (99%)	0.23	8 (3%) 44 26	47, 68, 85, 89	0
5	AE	151/162 (93%)	-0.08	0 100 100	49, 67, 94, 107	0
5	CE	151/162 (93%)	0.24	3 (1%) 65 41	53, 75, 94, 100	0
6	AF	101/101 (100%)	-0.04	0 100 100	54, 69, 84, 98	0
6	CF	101/101 (100%)	0.04	0 100 100	49, 73, 83, 98	0
7	AG	155/156 (99%)	0.38	10 (6%) 25 17	62, 82, 107, 124	0
7	CG	154/156 (98%)	0.47	9 (5%) 29 18	69, 92, 116, 124	0
8	AH	138/138 (100%)	0.04	2 (1%) 73 49	54, 71, 82, 96	0
8	CH	138/138 (100%)	0.25	2 (1%) 73 49	55, 75, 87, 97	0
9	AI	127/128 (99%)	0.69	10 (7%) 18 13	57, 99, 123, 126	0
9	CI	127/128 (99%)	0.93	15 (11%) 9 7	72, 106, 123, 129	0
10	AJ	99/105 (94%)	1.18	15 (15%) 5 5	69, 108, 130, 130	0
10	CJ	99/105 (94%)	0.98	12 (12%) 8 7	79, 115, 136, 143	0
11	AK	116/129 (89%)	0.08	4 (3%) 48 29	53, 67, 89, 107	0
11	CK	119/129 (92%)	0.19	6 (5%) 34 20	56, 76, 99, 114	0
12	AL	125/132 (94%)	0.38	5 (4%) 42 25	49, 63, 80, 103	0
12	CL	125/132 (94%)	0.36	5 (4%) 42 25	51, 71, 83, 99	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	122/126 (96%)	0.51	12 (9%) 13 9	63, 87, 97, 102	0
13	CM	118/126 (93%)	0.86	15 (12%) 8 7	77, 100, 114, 120	0
14	AN	60/61 (98%)	0.64	6 (10%) 12 9	52, 77, 91, 97	0
14	CN	60/61 (98%)	1.27	8 (13%) 7 6	75, 92, 101, 105	0
15	AO	88/89 (98%)	0.13	1 (1%) 78 54	47, 65, 82, 93	0
15	CO	88/89 (98%)	0.09	2 (2%) 61 38	50, 70, 87, 92	0
16	AP	84/88 (95%)	0.20	0 100 100	50, 68, 95, 109	0
16	CP	84/88 (95%)	0.44	4 (4%) 35 21	55, 66, 85, 109	0
17	AQ	100/105 (95%)	0.18	1 (1%) 79 56	53, 69, 84, 88	0
17	CQ	100/105 (95%)	0.25	2 (2%) 65 41	59, 73, 91, 94	0
18	AR	70/88 (79%)	0.38	3 (4%) 40 23	49, 68, 94, 100	0
18	CR	70/88 (79%)	0.07	3 (4%) 40 23	56, 74, 99, 104	0
19	AS	79/93 (84%)	0.71	7 (8%) 15 11	63, 90, 110, 115	0
19	CS	79/93 (84%)	1.02	9 (11%) 10 7	91, 111, 132, 138	0
20	AT	99/106 (93%)	0.72	8 (8%) 18 13	54, 75, 104, 110	0
20	CT	99/106 (93%)	0.71	7 (7%) 22 15	63, 76, 111, 114	0
21	AU	25/27 (92%)	1.00	1 (4%) 42 25	74, 82, 90, 95	0
21	CU	25/27 (92%)	0.99	2 (8%) 18 13	72, 93, 105, 109	0
22	AV	10/30 (33%)	1.13	3 (30%) 1 2	51, 66, 125, 128	0
22	CV	10/30 (33%)	1.06	3 (30%) 1 2	65, 81, 134, 138	0
23	AW	74/75 (98%)	0.15	3 (4%) 41 24	49, 117, 149, 154	0
23	CW	74/75 (98%)	0.40	3 (4%) 41 24	79, 129, 148, 165	0
24	AX	77/77 (100%)	-0.01	1 (1%) 75 51	35, 85, 115, 128	0
25	AY	75/75 (100%)	0.46	8 (10%) 11 9	62, 157, 189, 191	0
25	CY	75/75 (100%)	0.69	8 (10%) 11 9	76, 170, 192, 197	0
26	AZ	1/6 (16%)	0.09	0 100 100	64, 64, 64, 64	0
26	CZ	1/6 (16%)	-0.26	0 100 100	91, 91, 91, 91	0
27	BA	2789/2915 (95%)	-0.34	57 (2%) 65 41	19, 44, 164, 200	0
27	DA	2775/2915 (95%)	0.10	85 (3%) 51 31	30, 72, 170, 200	0
28	BB	119/122 (97%)	0.19	8 (6%) 24 16	36, 70, 127, 168	0
28	DB	119/122 (97%)	1.82	40 (33%) 1 1	109, 142, 170, 179	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
29	BC	191/229 (83%)	1.67	69 (36%) 1 1	103, 169, 180, 186	0
29	DC	191/229 (83%)	1.37	42 (21%) 2 3	125, 170, 183, 186	0
30	BD	272/276 (98%)	-0.01	10 (3%) 45 27	18, 41, 61, 73	0
30	DD	272/276 (98%)	0.11	6 (2%) 62 39	31, 52, 69, 81	0
31	BE	205/206 (99%)	-0.05	4 (1%) 65 41	16, 42, 76, 94	0
31	DE	205/206 (99%)	0.55	13 (6%) 26 17	44, 80, 112, 119	0
32	BF	206/210 (98%)	-0.09	4 (1%) 66 42	17, 46, 110, 129	0
32	DF	208/210 (99%)	0.33	3 (1%) 73 49	40, 69, 120, 132	0
33	BG	181/182 (99%)	0.29	6 (3%) 49 29	49, 74, 102, 119	0
33	DG	181/182 (99%)	0.62	10 (5%) 30 19	75, 101, 117, 125	0
34	BH	161/180 (89%)	0.34	10 (6%) 26 17	39, 65, 81, 95	0
34	DH	160/180 (88%)	1.14	24 (15%) 5 5	106, 129, 153, 161	0
35	BI	146/148 (98%)	1.36	35 (23%) 2 2	57, 134, 150, 159	0
35	DI	146/148 (98%)	0.77	13 (8%) 15 11	62, 107, 139, 150	0
36	BN	139/140 (99%)	-0.01	0 100 100	23, 43, 67, 73	0
36	DN	139/140 (99%)	0.70	13 (9%) 14 10	69, 86, 106, 108	0
37	BO	122/122 (100%)	-0.26	0 100 100	22, 44, 60, 67	0
37	DO	122/122 (100%)	0.31	2 (1%) 70 46	47, 72, 80, 86	0
38	BP	146/150 (97%)	0.63	17 (11%) 9 7	17, 60, 91, 121	0
38	DP	146/150 (97%)	1.04	28 (19%) 3 3	45, 82, 103, 126	0
39	BQ	139/141 (98%)	0.02	2 (1%) 73 49	29, 47, 70, 82	0
39	DQ	138/141 (97%)	0.99	23 (16%) 4 4	58, 88, 107, 136	0
40	BR	117/118 (99%)	0.05	4 (3%) 48 29	17, 37, 59, 66	0
40	DR	117/118 (99%)	0.45	9 (7%) 19 14	39, 64, 81, 88	0
41	BS	99/112 (88%)	0.62	12 (12%) 8 7	40, 65, 82, 91	0
41	DS	99/112 (88%)	1.21	23 (23%) 2 3	71, 93, 106, 109	0
42	BT	138/146 (94%)	0.39	7 (5%) 33 20	27, 53, 108, 143	0
42	DT	138/146 (94%)	0.67	10 (7%) 21 15	64, 79, 136, 142	0
43	BU	117/118 (99%)	-0.10	1 (0%) 81 58	20, 37, 59, 86	0
43	DU	117/118 (99%)	0.47	10 (8%) 16 12	48, 80, 111, 120	0
44	BV	101/101 (100%)	0.00	1 (0%) 79 56	18, 49, 68, 74	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	DV	101/101 (100%)	0.44	7 (6%) 23 15	54, 100, 114, 122	0
45	BW	113/113 (100%)	-0.25	1 (0%) 81 58	21, 34, 64, 102	0
45	DW	113/113 (100%)	0.12	1 (0%) 81 58	39, 61, 93, 118	0
46	BX	93/96 (96%)	-0.01	1 (1%) 78 54	31, 45, 69, 76	0
46	DX	93/96 (96%)	0.30	4 (4%) 40 23	39, 66, 79, 85	0
47	BY	88/110 (80%)	0.62	8 (9%) 15 11	41, 58, 79, 87	0
47	DY	101/110 (91%)	1.34	23 (22%) 2 3	62, 83, 144, 153	0
48	BZ	177/206 (85%)	0.78	28 (15%) 5 5	52, 85, 159, 164	0
48	DZ	177/206 (85%)	1.31	32 (18%) 3 4	93, 123, 178, 184	0
49	B0	84/85 (98%)	0.28	5 (5%) 27 17	27, 49, 71, 85	0
49	D0	84/85 (98%)	0.82	8 (9%) 14 10	66, 82, 96, 104	0
50	B1	94/98 (95%)	0.11	3 (3%) 50 30	28, 49, 80, 91	0
50	D1	94/98 (95%)	0.42	2 (2%) 63 39	40, 62, 94, 101	0
51	B2	71/72 (98%)	0.13	2 (2%) 55 33	37, 62, 93, 106	0
51	D2	71/72 (98%)	0.19	1 (1%) 73 49	59, 78, 98, 117	0
52	B3	60/60 (100%)	0.09	0 100 100	27, 44, 69, 103	0
52	D3	60/60 (100%)	0.70	1 (1%) 69 44	70, 88, 111, 119	0
53	B4	49/71 (69%)	0.87	10 (20%) 3 3	72, 97, 116, 119	0
53	D4	49/71 (69%)	0.93	7 (14%) 6 6	100, 115, 120, 121	0
54	B5	59/60 (98%)	0.35	5 (8%) 16 12	21, 38, 93, 115	0
54	D5	59/60 (98%)	0.52	4 (6%) 23 16	46, 62, 116, 136	0
55	B6	48/54 (88%)	1.10	7 (14%) 6 5	29, 58, 71, 90	0
55	D6	46/54 (85%)	1.71	17 (36%) 1 1	50, 81, 91, 101	0
56	B7	49/49 (100%)	-0.00	2 (4%) 41 24	20, 32, 77, 90	0
56	D7	49/49 (100%)	0.19	3 (6%) 27 17	36, 47, 84, 92	0
57	B8	64/65 (98%)	0.69	7 (10%) 10 8	26, 44, 62, 99	0
57	D8	64/65 (98%)	1.23	11 (17%) 4 4	51, 66, 85, 109	0
58	B9	36/37 (97%)	-0.02	0 100 100	15, 45, 57, 59	0
58	D9	36/37 (97%)	1.25	9 (25%) 2 2	79, 94, 99, 102	0
59	CX	77/77 (100%)	0.14	1 (1%) 75 51	63, 100, 127, 140	0
All	All	21180/22202 (95%)	0.27	1187 (5%) 30 19	15, 72, 152, 200	0

All (1187) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
57	D8	65	GLU	10.0
35	BI	94	ALA	10.0
54	D5	2	ALA	9.5
28	DB	49	C	9.0
34	DH	170	ARG	8.6
28	DB	27	C	8.3
48	DZ	112	ALA	8.2
48	DZ	110	VAL	8.0
27	DA	896	A	7.4
53	B4	56	GLU	7.3
34	DH	171	LEU	7.3
11	CK	129	SER	7.1
27	BA	2116	G	6.8
13	CM	84	ILE	6.7
48	DZ	109	GLY	6.7
38	DP	51	PHE	6.3
42	DT	2	ASN	6.1
44	BV	36	PRO	6.1
38	DP	27	HIS	6.1
25	CY	33	G	6.0
31	DE	76	ARG	6.0
42	BT	1	MET	5.9
48	DZ	114	GLY	5.9
29	BC	49	ILE	5.9
48	BZ	174	VAL	5.8
29	DC	139	ASN	5.8
47	DY	51	VAL	5.8
57	B8	64	TYR	5.7
48	BZ	119	ILE	5.7
48	BZ	169	THR	5.7
47	DY	65	ALA	5.6
31	BE	76	ARG	5.6
28	BB	88	C	5.6
48	DZ	174	VAL	5.5
41	DS	11	LYS	5.5
48	DZ	175	PRO	5.4
59	CX	1	C	5.4
53	B4	71	GLN	5.4
29	BC	139	ASN	5.3
57	D8	56	GLU	5.3
7	AG	81	GLY	5.3
7	AG	82	GLY	5.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
25	AY	33	G	5.3
27	DA	2802	G	5.2
48	DZ	176	PRO	5.2
1	CA	1030(B)	C	5.2
30	BD	34	VAL	5.1
57	D8	64	TYR	5.1
33	BG	35	GLU	5.0
7	AG	83	ALA	5.0
29	DC	57	ASN	5.0
49	B0	3	HIS	4.9
17	CQ	101	ARG	4.9
48	BZ	115	VAL	4.9
28	DB	31	C	4.9
27	DA	1026	U	4.9
27	DA	274	G	4.9
35	BI	121	LYS	4.8
4	CD	31	CYS	4.8
47	DY	61	ILE	4.8
2	CB	134	GLU	4.8
7	CG	2	ALA	4.8
48	BZ	172	ALA	4.8
48	DZ	149	LEU	4.7
29	BC	48	GLY	4.7
27	BA	92	A	4.7
27	DA	543	C	4.7
27	DA	1530	C	4.7
28	DB	76	G	4.7
48	DZ	116	LEU	4.7
35	BI	41	GLU	4.7
49	D0	3	HIS	4.6
29	BC	179	SER	4.6
27	BA	1531	C	4.6
9	CI	67	GLY	4.6
31	DE	132	HIS	4.6
41	DS	109	GLY	4.6
14	CN	14	PRO	4.6
48	BZ	117	GLN	4.6
30	DD	40	THR	4.5
49	B0	41	ARG	4.5
34	DH	168	PRO	4.5
50	D1	95	LEU	4.5
27	DA	1112	G	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	CB	133	LYS	4.4
27	DA	2892	A	4.4
4	AD	209	ARG	4.4
2	CB	215	LEU	4.4
2	AB	133	LYS	4.4
11	CK	127	LYS	4.4
38	BP	51	PHE	4.4
39	DQ	139	GLU	4.4
27	DA	92	A	4.4
28	DB	29	A	4.3
47	DY	79	CYS	4.3
1	AA	1280	A	4.3
34	DH	169	VAL	4.3
20	CT	10	LEU	4.3
35	BI	143	SER	4.2
55	D6	21	TYR	4.2
27	BA	652	C	4.2
35	BI	92	VAL	4.2
55	D6	13	CYS	4.2
22	CV	1	A	4.2
1	CA	1001(A)	G	4.2
13	AM	6	GLY	4.2
13	AM	121	LYS	4.2
30	BD	244	ARG	4.2
29	BC	165	ASN	4.2
39	DQ	1	MET	4.2
48	DZ	178	ASP	4.1
48	DZ	107	PRO	4.1
48	DZ	115	VAL	4.1
53	D4	81	VAL	4.1
12	AL	44	LYS	4.1
41	DS	54	LEU	4.1
48	BZ	177	GLU	4.1
35	BI	95	LYS	4.1
28	DB	88	C	4.1
2	CB	131	PRO	4.1
29	BC	50	ASP	4.1
29	BC	56	GLN	4.1
2	CB	137	ARG	4.1
27	DA	651	G	4.1
1	CA	99	U	4.1
14	CN	15	LYS	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
35	BI	117	GLU	4.0
54	B5	60	VAL	4.0
41	BS	11	LYS	4.0
4	AD	31	CYS	4.0
20	AT	12	ALA	4.0
31	DE	77	ILE	4.0
38	DP	19	VAL	4.0
28	DB	48	A	4.0
28	DB	57	A	4.0
29	BC	62	VAL	3.9
20	CT	99	LEU	3.9
27	BA	275	G	3.9
29	BC	34	THR	3.9
38	DP	110	TYR	3.9
57	D8	35	GLN	3.9
1	CA	1281	U	3.9
3	CC	155	GLY	3.9
1	AA	89	C	3.9
29	BC	206	GLY	3.9
48	DZ	113	GLY	3.9
55	D6	31	PRO	3.9
29	BC	107	TRP	3.9
9	AI	111	ARG	3.9
3	AC	207	VAL	3.9
27	BA	2179	C	3.9
38	BP	43	GLY	3.8
55	B6	53	LYS	3.8
29	BC	166	ASP	3.8
48	BZ	120	HIS	3.8
35	BI	97	ILE	3.8
34	DH	35	VAL	3.8
1	CA	1030(C)	G	3.8
41	DS	12	PHE	3.8
47	DY	2	ARG	3.8
29	DC	50	ASP	3.8
48	BZ	178	ASP	3.8
47	BY	3	VAL	3.8
55	B6	42	TRP	3.8
27	BA	90	U	3.8
1	CA	1397	C	3.8
9	CI	12	GLU	3.8
29	BC	121	GLY	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	AG	84	ASN	3.8
48	DZ	173	VAL	3.8
10	CJ	46	ARG	3.8
29	BC	164	ARG	3.8
1	AA	82	U	3.8
31	BE	205	ALA	3.7
30	DD	34	VAL	3.7
30	DD	38	LYS	3.7
54	B5	59	GLU	3.7
2	CB	222	ILE	3.7
12	AL	25	LYS	3.7
28	BB	89	G	3.7
1	CA	1125	U	3.7
41	BS	33	LYS	3.7
23	AW	2	G	3.7
27	BA	1529	G	3.7
9	CI	62	TYR	3.7
47	DY	3	VAL	3.7
27	BA	1178	C	3.7
8	CH	1	MET	3.7
47	DY	57	GLN	3.7
11	CK	124	LYS	3.7
53	D4	56	GLU	3.6
41	DS	14	VAL	3.6
1	AA	1130	A	3.6
41	DS	99	LYS	3.6
29	DC	179	SER	3.6
1	AA	306	G	3.6
27	BA	508	G	3.6
27	DA	2192	G	3.6
39	DQ	140	ALA	3.6
2	AB	134	GLU	3.6
48	BZ	118	GLU	3.6
29	DC	53	ARG	3.6
40	DR	11	ASN	3.6
27	DA	1529	G	3.6
1	CA	1286	A	3.6
55	D6	8	LYS	3.6
29	DC	49	ILE	3.6
28	DB	60	C	3.6
48	DZ	169	THR	3.6
39	DQ	141	GLN	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
10	AJ	59	SER	3.6
28	BB	90	A	3.5
28	DB	56	G	3.5
34	DH	120	GLY	3.5
28	DB	12	C	3.5
28	DB	28	C	3.5
29	BC	140	PRO	3.5
55	D6	53	LYS	3.5
3	CC	15	THR	3.5
36	DN	43	THR	3.5
48	DZ	106	THR	3.5
10	AJ	62	HIS	3.5
47	BY	49	VAL	3.5
47	DY	49	VAL	3.5
32	BF	25	PRO	3.5
1	AA	1456	G	3.5
27	BA	2115	G	3.5
25	AY	16	C	3.5
27	BA	1530	C	3.5
48	BZ	145	ILE	3.5
38	DP	52	GLU	3.5
29	DC	148	ASN	3.5
29	DC	110	PHE	3.5
55	B6	23	THR	3.5
1	CA	1150	U	3.5
38	DP	64	LYS	3.5
29	BC	47	LEU	3.5
39	DQ	136	ALA	3.5
27	BA	880	G	3.5
34	BH	167	GLU	3.4
57	D8	48	PHE	3.4
41	DS	32	LEU	3.4
35	BI	88	ILE	3.4
27	BA	543	C	3.4
34	DH	33	LEU	3.4
35	DI	116	LEU	3.4
42	DT	25	GLY	3.4
29	BC	25	ALA	3.4
53	B4	77	THR	3.4
20	AT	74	LYS	3.4
28	DB	47	C	3.4
55	D6	23	THR	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
25	CY	17	G	3.4
19	CS	80	TYR	3.4
36	DN	78	TYR	3.4
13	CM	85	GLY	3.4
29	DC	26	ALA	3.4
29	BC	40	THR	3.4
1	CA	1126	U	3.4
25	AY	34	U	3.4
10	CJ	59	SER	3.4
34	DH	114	VAL	3.4
41	DS	30	ARG	3.4
27	BA	2112	G	3.4
29	BC	45	ALA	3.4
40	BR	7	GLY	3.4
35	BI	138	ILE	3.4
27	BA	1026	U	3.3
27	DA	2796	U	3.3
55	D6	12	GLU	3.3
49	B0	2	ALA	3.3
35	BI	120	ILE	3.3
27	DA	2308	G	3.3
28	DB	86	G	3.3
13	CM	102	ARG	3.3
40	DR	8	ARG	3.3
9	CI	109	VAL	3.3
10	AJ	55	LYS	3.3
27	DA	2757	A	3.3
1	AA	81	U	3.3
28	BB	1	U	3.3
25	CY	16	C	3.3
48	BZ	110	VAL	3.3
2	AB	132	LYS	3.3
55	D6	43	CYS	3.3
27	DA	1494	A	3.3
28	DB	13	A	3.3
33	DG	2	PRO	3.3
42	DT	3	ARG	3.3
48	DZ	111	ARG	3.3
38	DP	43	GLY	3.3
27	DA	2147	G	3.3
28	DB	51	G	3.3
41	BS	12	PHE	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
22	AV	10	U	3.3
27	DA	90	U	3.3
41	DS	61	ASN	3.3
55	D6	42	TRP	3.3
28	DB	6	C	3.3
4	CD	209	ARG	3.2
27	BA	10	G	3.2
27	DA	2116	G	3.2
28	DB	85	G	3.2
28	DB	90	A	3.2
30	BD	273	ARG	3.2
27	DA	2752	C	3.2
35	BI	91	SER	3.2
48	BZ	173	VAL	3.2
35	DI	4	ILE	3.2
28	DB	50	G	3.2
48	BZ	141	SER	3.2
53	B4	79	GLY	3.2
55	D6	26	ASN	3.2
34	DH	157	TYR	3.2
57	D8	63	PRO	3.2
49	B0	74	ARG	3.2
54	D5	29	THR	3.2
27	BA	1740	G	3.2
48	DZ	77	LYS	3.2
27	BA	2402	C	3.2
29	DC	47	LEU	3.2
35	DI	122	GLU	3.2
55	B6	24	GLU	3.2
48	BZ	175	PRO	3.2
14	AN	2	ALA	3.2
54	B5	2	ALA	3.2
27	DA	158	U	3.1
19	CS	82	GLY	3.1
1	CA	1130	A	3.1
27	DA	279	C	3.1
13	CM	87	TYR	3.1
13	AM	84	ILE	3.1
29	DC	56	GLN	3.1
47	DY	60	PHE	3.1
29	DC	51	PRO	3.1
19	AS	80	TYR	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
38	BP	110	TYR	3.1
48	BZ	108	ALA	3.1
48	DZ	117	GLN	3.1
10	AJ	88	LEU	3.1
1	CA	1531	A	3.1
10	AJ	48	THR	3.1
27	BA	896	A	3.1
29	DC	144	THR	3.1
29	DC	206	GLY	3.1
1	AA	1129	C	3.1
9	AI	110	GLU	3.1
27	DA	2896	C	3.1
29	BC	110	PHE	3.1
29	BC	224	ILE	3.1
20	CT	12	ALA	3.1
38	DP	62	LEU	3.1
36	DN	73	THR	3.1
38	BP	26	GLY	3.1
56	D7	47	ARG	3.1
27	BA	2117	A	3.1
3	CC	196	LEU	3.0
57	D8	51	ALA	3.0
38	DP	77	ARG	3.0
30	BD	32	SER	3.0
48	DZ	136	ILE	3.0
29	DC	45	ALA	3.0
29	DC	52	ARG	3.0
24	AX	1	C	3.0
16	CP	35	LYS	3.0
31	DE	75	VAL	3.0
1	CA	723	U	3.0
1	CA	1370	G	3.0
28	BB	119	G	3.0
7	AG	85	TYR	3.0
9	CI	128	ARG	3.0
30	BD	42	GLY	3.0
13	AM	7	VAL	3.0
22	CV	2	A	3.0
27	DA	2117	A	3.0
35	BI	21	VAL	3.0
1	CA	1030	C	3.0
55	D6	10	LEU	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
35	DI	113	ARG	3.0
39	BQ	136	ALA	3.0
41	BS	89	ARG	3.0
42	DT	130	ALA	3.0
56	D7	48	LYS	3.0
27	DA	508	G	3.0
57	B8	35	GLN	3.0
29	DC	165	ASN	3.0
29	BC	207	THR	3.0
10	AJ	98	ILE	3.0
33	BG	2	PRO	3.0
41	BS	30	ARG	3.0
35	BI	110	ASP	3.0
13	CM	119	GLY	3.0
34	DH	61	HIS	3.0
48	DZ	79	ARG	2.9
1	AA	80	G	2.9
1	CA	1139	G	2.9
12	CL	125	ALA	2.9
1	AA	1503	A	2.9
40	BR	3	HIS	2.9
1	CA	92	C	2.9
55	D6	20	ASN	2.9
40	DR	9	LYS	2.9
57	D8	34	TRP	2.9
29	BC	89	ALA	2.9
43	DU	47	TYR	2.9
41	BS	14	VAL	2.9
41	BS	98	VAL	2.9
9	AI	30	GLY	2.9
27	DA	879	G	2.9
28	DB	87	G	2.9
58	D9	17	ILE	2.9
28	DB	58	A	2.9
29	BC	64	LEU	2.9
38	DP	50	ARG	2.9
1	CA	1116	C	2.9
39	BQ	139	GLU	2.9
57	B8	65	GLU	2.9
29	DC	60	GLY	2.9
34	BH	48	GLY	2.9
50	D1	96	LYS	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
42	BT	27	THR	2.9
1	AA	1124	G	2.9
1	AA	1224	G	2.9
1	CA	77	G	2.9
1	CA	1002	G	2.9
25	CY	35	G	2.9
27	BA	879	G	2.9
27	DA	2893	G	2.9
28	BB	87	G	2.9
53	B4	78	GLU	2.9
1	CA	1129	C	2.9
11	CK	25	TYR	2.9
29	BC	143	GLY	2.9
35	BI	90	GLY	2.9
38	DP	40	SER	2.9
29	DC	177	LYS	2.9
30	BD	38	LYS	2.9
36	DN	109	LYS	2.9
39	DQ	20	ALA	2.9
47	DY	48	ALA	2.9
30	BD	237	GLU	2.9
52	D3	11	SER	2.8
29	BC	178	ALA	2.8
47	BY	77	PRO	2.8
13	CM	7	VAL	2.8
9	CI	18	PHE	2.8
34	BH	85	LYS	2.8
32	BF	24	LEU	2.8
40	DR	10	LEU	2.8
28	DB	45	A	2.8
14	CN	2	ALA	2.8
49	D0	2	ALA	2.8
1	CA	1124	G	2.8
25	CY	52	G	2.8
27	DA	2795	G	2.8
28	DB	74	U	2.8
28	DB	89	G	2.8
1	CA	1027	C	2.8
34	DH	60	ARG	2.8
38	DP	65	ARG	2.8
32	BF	134	GLY	2.8
35	BI	25	TYR	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
53	B4	69	TYR	2.8
51	B2	72	ALA	2.8
39	DQ	85	LYS	2.8
55	B6	12	GLU	2.8
27	DA	2310	A	2.8
27	DA	2801	A	2.8
27	DA	2895	U	2.8
27	DA	880	G	2.8
8	CH	135	CYS	2.8
9	AI	10	ARG	2.8
14	CN	31	ARG	2.8
7	AG	80	VAL	2.8
12	AL	22	PRO	2.8
19	AS	4	SER	2.8
29	DC	58	VAL	2.8
50	B1	95	LEU	2.8
32	BF	23	ASP	2.8
33	DG	29	TRP	2.8
38	DP	28	GLY	2.8
1	AA	723	U	2.8
20	AT	73	HIS	2.8
2	AB	144	ARG	2.8
18	CR	84	LYS	2.8
27	BA	2474	C	2.8
29	BC	170	ALA	2.8
13	CM	97	PRO	2.8
27	DA	171	G	2.8
20	AT	10	LEU	2.8
2	CB	163	PHE	2.7
29	DC	61	THR	2.8
11	AK	52	GLY	2.7
29	BC	109	ASP	2.7
29	DC	48	GLY	2.7
29	DC	109	ASP	2.7
29	BC	26	ALA	2.7
42	DT	94	ALA	2.7
4	CD	9	CYS	2.7
41	DS	98	VAL	2.7
29	BC	174	PRO	2.7
28	DB	42	C	2.7
30	BD	12	SER	2.7
31	BE	77	ILE	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	CA	1033	G	2.7
25	AY	35	G	2.7
27	BA	1171	G	2.7
27	DA	2125	G	2.7
27	DA	2193	G	2.7
2	AB	8	LYS	2.7
35	DI	87	LYS	2.7
43	DU	19	LYS	2.7
41	DS	102	ALA	2.7
42	DT	131	ALA	2.7
48	DZ	163	ALA	2.7
48	DZ	172	ALA	2.7
2	AB	196	LEU	2.7
27	BA	158	U	2.7
27	DA	1544	A	2.7
30	BD	55	GLY	2.7
1	AA	984	C	2.7
27	BA	2136	C	2.7
27	DA	2136	C	2.7
29	DC	175	VAL	2.7
1	CA	104	G	2.7
28	DB	23	G	2.7
2	AB	201	ILE	2.7
3	CC	186	PHE	2.7
42	DT	1	MET	2.7
35	BI	99	GLU	2.7
48	BZ	142	GLY	2.7
48	DZ	177	GLU	2.7
12	CL	25	LYS	2.7
31	DE	133	LYS	2.7
43	DU	93	LYS	2.7
48	BZ	148	SER	2.7
1	AA	1125	U	2.7
27	DA	1113	U	2.7
28	DB	14	U	2.7
22	AV	1	A	2.7
28	DB	25	A	2.7
14	CN	34	TYR	2.7
15	CO	69	TYR	2.7
29	BC	35	ALA	2.7
34	DH	165	ALA	2.7
41	DS	100	ALA	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	CB	136	VAL	2.7
3	CC	94	LEU	2.7
20	CT	24	LEU	2.7
48	BZ	116	LEU	2.7
58	D9	20	HIS	2.7
10	CJ	39	PRO	2.7
27	DA	1493	C	2.7
27	DA	2146	C	2.7
28	DB	4	C	2.7
38	DP	78	PRO	2.7
41	DS	15	ARG	2.7
33	DG	35	GLU	2.7
43	DU	15	LYS	2.7
29	DC	215	THR	2.7
1	CA	1030(A)	G	2.7
48	DZ	152	SER	2.7
3	CC	193	TYR	2.7
10	AJ	40	LEU	2.7
19	CS	41	VAL	2.7
44	DV	20	LEU	2.7
29	BC	148	ASN	2.7
34	BH	8	PRO	2.6
9	CI	111	ARG	2.6
19	CS	81	ARG	2.6
58	D9	2	LYS	2.6
31	DE	163	GLU	2.6
35	BI	135	GLU	2.6
7	CG	83	ALA	2.6
41	BS	54	LEU	2.6
39	DQ	137	TYR	2.6
42	DT	100	TYR	2.6
1	CA	1117	G	2.6
9	CI	66	ARG	2.6
27	BA	2793	G	2.6
19	CS	10	PHE	2.6
44	DV	36	PRO	2.6
27	DA	1033	U	2.6
7	CG	82	GLY	2.6
29	BC	60	GLY	2.6
1	CA	1503	A	2.6
9	CI	64	THR	2.6
47	DY	99	CYS	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
10	CJ	65	LEU	2.6
31	DE	63	LEU	2.6
35	BI	145	VAL	2.6
1	AA	1027	C	2.6
27	DA	2804	C	2.6
29	BC	54	SER	2.6
34	BH	111	HIS	2.6
35	DI	138	ILE	2.6
40	DR	2	ARG	2.6
41	DS	33	LYS	2.6
29	BC	201	PRO	2.6
47	DY	56	PRO	2.6
47	DY	77	PRO	2.6
39	DQ	113	GLN	2.6
39	DQ	19	GLY	2.6
39	DQ	23	GLY	2.6
43	BU	118	GLY	2.6
1	AA	1126	U	2.6
20	AT	99	LEU	2.6
33	BG	3	LEU	2.6
29	BC	142	ALA	2.6
36	DN	3	THR	2.6
19	AS	78	ARG	2.6
27	BA	2173	A	2.6
27	DA	2062	A	2.6
27	DA	2801(A)	A	2.6
42	BT	3	ARG	2.6
44	DV	21	ARG	2.6
4	AD	208	SER	2.6
11	CK	125	PHE	2.6
29	DC	140	PRO	2.6
1	CA	1249	C	2.6
35	BI	11	ASN	2.6
42	BT	4	GLY	2.6
42	BT	55	ASN	2.6
3	CC	178	LEU	2.6
29	DC	75	LEU	2.6
35	BI	116	LEU	2.6
48	BZ	96	GLU	2.6
9	CI	14	VAL	2.6
29	DC	62	VAL	2.6
35	BI	142	VAL	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	CB	144	ARG	2.6
18	AR	71	LYS	2.6
20	AT	21	LYS	2.6
38	DP	33	ARG	2.6
35	DI	79	ILE	2.6
10	CJ	47	PHE	2.6
5	CE	77	PRO	2.6
38	DP	24	GLY	2.6
45	BW	60	ASN	2.6
54	D5	58	LEU	2.6
27	BA	2145	C	2.6
27	DA	1119	C	2.6
29	DC	194	ARG	2.6
53	B4	81	VAL	2.6
41	BS	99	LYS	2.6
25	CY	34	U	2.5
46	DX	5	TYR	2.5
2	AB	131	PRO	2.5
36	DN	44	PRO	2.5
47	BY	82	PRO	2.5
47	DY	76	CYS	2.5
20	CT	11	SER	2.5
13	CM	100	GLY	2.5
48	DZ	159	GLY	2.5
23	CW	2	G	2.5
27	DA	2319	G	2.5
28	BB	86	G	2.5
1	CA	977	A	2.5
12	AL	23	ALA	2.5
48	DZ	108	ALA	2.5
1	AA	1452	C	2.5
27	BA	2804	C	2.5
29	DC	220	PRO	2.5
14	CN	38	GLY	2.5
35	BI	30	LEU	2.5
10	CJ	66	ARG	2.5
29	BC	160	ARG	2.5
29	BC	177	LYS	2.5
49	B0	55	ARG	2.5
58	D9	4	ARG	2.5
54	D5	57	VAL	2.5
47	DY	44	ILE	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	CA	1183	A	2.5
27	BA	529	A	2.5
27	BA	2751	G	2.5
38	BP	27	HIS	2.5
1	CA	979	C	2.5
27	BA	2174	C	2.5
27	DA	34	C	2.5
27	DA	2803	C	2.5
38	DP	44	GLY	2.5
42	BT	92	GLY	2.5
47	DY	10	GLY	2.5
19	AS	56	GLN	2.5
29	BC	211	SER	2.5
10	AJ	75	ILE	2.5
34	DH	136	ILE	2.5
9	AI	64	THR	2.5
5	CE	12	LEU	2.5
29	BC	59	ARG	2.5
38	DP	61	ARG	2.5
41	BS	15	ARG	2.5
50	B1	26	ARG	2.5
1	AA	1183	A	2.5
7	CG	81	GLY	2.5
21	AU	2	GLY	2.5
27	BA	1544	A	2.5
27	DA	899	A	2.5
29	BC	43	VAL	2.5
1	AA	1026	G	2.5
20	AT	11	SER	2.5
47	BY	78	ALA	2.5
48	DZ	151	ALA	2.5
10	AJ	64	GLU	2.5
27	DA	2799	C	2.5
34	DH	167	GLU	2.5
11	AK	81	ASP	2.5
14	AN	61	TRP	2.5
29	BC	144	THR	2.5
7	AG	5	ARG	2.5
38	BP	148	LEU	2.5
38	DP	59	LEU	2.5
48	BZ	111	ARG	2.5
9	CI	58	HIS	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
29	BC	74	VAL	2.5
31	DE	72	VAL	2.5
54	B5	57	VAL	2.5
35	BI	146	ALA	2.4
4	AD	26	CYS	2.4
7	CG	77	SER	2.4
10	AJ	6	ILE	2.4
27	BA	2119	A	2.4
13	CM	99	ARG	2.4
20	CT	8	ARG	2.4
53	B4	54	LYS	2.4
1	AA	1001(A)	G	2.4
27	DA	2894	G	2.4
34	BH	158	HIS	2.4
49	D0	73	GLY	2.4
10	AJ	54	PHE	2.4
36	DN	74	ARG	2.4
38	BP	64	LYS	2.4
46	BX	33	LYS	2.4
47	DY	86	ARG	2.4
1	CA	1287	A	2.4
53	B4	76	ASP	2.4
13	AM	85	GLY	2.4
11	CK	128	ALA	2.4
1	CA	1036	G	2.4
2	AB	214	ILE	2.4
2	AB	222	ILE	2.4
3	AC	14	ILE	2.4
29	BC	204	ALA	2.4
27	BA	2120	G	2.4
28	DB	107	G	2.4
35	BI	79	ILE	2.4
29	BC	120	MET	2.4
9	CI	110	GLU	2.4
38	DP	41	ARG	2.4
57	B8	48	PHE	2.4
18	AR	79	LEU	2.4
41	DS	58	LEU	2.4
33	BG	87	PRO	2.4
16	CP	32	TYR	2.4
10	CJ	32	ALA	2.4
1	AA	1447	A	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	AA	980	C	2.4
23	AW	16	C	2.4
25	CY	53	U	2.4
27	DA	2145	C	2.4
34	DH	34	GLU	2.4
40	DR	4	LEU	2.4
47	DY	52	SER	2.4
27	BA	2131	G	2.4
27	BA	2160	G	2.4
27	DA	1044	G	2.4
33	DG	28	VAL	2.4
34	DH	144	VAL	2.4
2	CB	211	ILE	2.4
7	CG	85	TYR	2.4
9	AI	62	TYR	2.4
29	BC	55	ASP	2.4
30	BD	41	GLY	2.4
29	DC	170	ALA	2.4
35	BI	112	LYS	2.4
41	DS	62	LYS	2.4
53	D4	85	GLN	2.4
9	AI	18	PHE	2.4
35	DI	140	LEU	2.4
57	B8	32	LEU	2.4
14	AN	8	GLU	2.4
22	CV	3	A	2.4
27	BA	2114	A	2.4
27	BA	362	U	2.4
53	B4	67	PRO	2.4
55	D6	52	VAL	2.4
1	CA	1325	C	2.3
1	CA	1362	C	2.3
3	AC	165	THR	2.3
28	DB	30	C	2.3
12	CL	26	GLY	2.3
29	BC	21	THR	2.3
47	BY	102	CYS	2.4
10	CJ	55	LYS	2.3
18	AR	84	LYS	2.3
29	BC	53	ARG	2.3
34	BH	60	ARG	2.3
1	CA	1003	G	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
23	AW	72	G	2.3
27	DA	1171	G	2.3
27	DA	2891	G	2.3
3	AC	178	LEU	2.3
3	CC	175	LEU	2.3
4	CD	19	LEU	2.3
19	CS	15	LEU	2.3
36	DN	67	LEU	2.3
41	DS	73	LEU	2.3
48	BZ	162	LEU	2.3
29	BC	214	VAL	2.3
11	AK	11	LYS	2.3
56	B7	48	LYS	2.3
57	B8	5	LYS	2.3
29	BC	173	ALA	2.3
35	BI	133	HIS	2.3
41	BS	102	ALA	2.3
1	CA	5	U	2.3
1	CA	1115	C	2.3
19	CS	5	LEU	2.3
13	AM	101	GLN	2.3
55	D6	24	GLU	2.3
58	D9	28	GLU	2.3
1	CA	855	G	2.3
1	CA	1185	G	2.3
9	AI	41	VAL	2.3
27	DA	100	G	2.3
29	BC	41	VAL	2.3
29	BC	145	VAL	2.3
38	BP	14	LYS	2.3
13	AM	102	ARG	2.3
35	DI	120	ILE	2.3
29	BC	215	THR	2.3
35	DI	115	ALA	2.3
42	DT	27	THR	2.3
45	DW	73	ALA	2.3
21	CU	18	TYR	2.3
38	BP	62	LEU	2.3
25	CY	54	U	2.3
27	BA	2132	U	2.3
29	BC	87	GLU	2.3
23	CW	16	C	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
27	DA	1178	C	2.3
38	BP	76	LYS	2.3
44	DV	37	VAL	2.3
3	CC	124	ILE	2.3
4	AD	2	GLY	2.3
8	AH	111	ILE	2.3
10	CJ	37	PRO	2.3
34	DH	29	PRO	2.3
35	DI	119	PRO	2.3
38	DP	109	GLY	2.3
49	D0	13	GLY	2.3
12	CL	23	ALA	2.3
43	DU	115	ALA	2.3
29	BC	216	THR	2.3
48	BZ	106	THR	2.3
1	CA	1202	G	2.3
19	AS	10	PHE	2.3
25	AY	17	G	2.3
27	BA	11	G	2.3
27	DA	272	G	2.3
4	CD	12	CYS	2.3
29	DC	187	ASP	2.3
39	DQ	138	ASP	2.3
43	DU	97	ASP	2.3
2	CB	8	LYS	2.3
19	AS	73	GLU	2.3
22	AV	2	A	2.3
30	DD	237	GLU	2.3
27	DA	2897	U	2.3
36	DN	108	PRO	2.3
48	BZ	170	ILE	2.3
53	D4	67	PRO	2.3
13	CM	6	GLY	2.3
35	BI	65	ALA	2.3
38	DP	31	ALA	2.3
46	DX	4	ALA	2.3
48	BZ	114	GLY	2.3
1	CA	856	C	2.3
4	AD	19	LEU	2.3
29	DC	217	THR	2.3
32	DF	24	LEU	2.3
35	BI	114	LEU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
19	CS	28	LYS	2.3
43	DU	33	ARG	2.3
19	CS	12	ASP	2.3
13	AM	8	GLU	2.2
1	CA	887	G	2.2
27	BA	1055	G	2.2
27	DA	656	G	2.2
33	DG	52	ILE	2.2
37	DO	30	ALA	2.2
10	CJ	85	LEU	2.2
27	DA	2758	A	2.2
29	BC	136	LEU	2.2
43	DU	98	LEU	2.2
3	AC	15	THR	2.2
10	CJ	42	THR	2.2
29	BC	163	PHE	2.2
35	BI	93	THR	2.2
12	CL	20	LYS	2.2
29	DC	141	LYS	2.2
35	BI	118	LYS	2.2
38	DP	29	LYS	2.2
38	DP	46	LYS	2.2
46	DX	33	LYS	2.2
1	AA	1397	C	2.2
7	AG	4	ARG	2.2
7	AG	32	ARG	2.2
21	CU	10	ARG	2.2
27	DA	1118	C	2.2
28	BB	91	C	2.2
58	D9	19	ARG	2.2
2	AB	239	VAL	2.2
13	CM	117	VAL	2.2
47	DY	27	VAL	2.2
48	DZ	140	VAL	2.2
39	DQ	127	ILE	2.2
14	AN	14	PRO	2.2
29	DC	181	PRO	2.2
38	BP	28	GLY	2.2
38	BP	147	LEU	2.2
57	D8	62	LEU	2.2
1	CA	70	G	2.2
27	DA	2805	G	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
28	DB	119	G	2.2
31	DE	64	LYS	2.2
31	DE	159	HIS	2.2
33	DG	64	THR	2.2
34	DH	111	HIS	2.2
38	DP	107	LYS	2.2
9	CI	9	ARG	2.2
28	DB	41	U	2.2
38	BP	16	ARG	2.2
38	BP	41	ARG	2.2
27	DA	6	A	2.2
2	CB	223	ILE	2.2
17	CQ	24	GLU	2.2
36	DN	139	GLU	2.2
13	CM	83	ASP	2.2
28	DB	91	C	2.2
29	BC	105	ASP	2.2
48	BZ	176	PRO	2.2
55	B6	41	PRO	2.2
9	AI	127	LYS	2.2
36	DN	83	LYS	2.2
41	DS	93	LYS	2.2
42	DT	8	LYS	2.2
55	D6	18	ARG	2.2
56	B7	49	ARG	2.2
35	BI	108	THR	2.2
1	CA	1086	U	2.2
33	DG	63	ILE	2.2
1	CA	971	G	2.2
27	BA	274	G	2.2
27	BA	2121	G	2.2
27	DA	900	A	2.2
27	DA	2833	G	2.2
33	BG	164	GLU	2.2
48	BZ	149	LEU	2.2
2	AB	218	ALA	2.2
13	CM	10	PRO	2.2
16	CP	84	ALA	2.2
31	DE	153	GLY	2.2
34	DH	102	ALA	2.2
42	BT	130	ALA	2.2
4	CD	22	LYS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
29	BC	141	LYS	2.2
48	BZ	122	ASP	2.2
29	DC	168	THR	2.2
39	DQ	21	THR	2.2
7	CG	61	VAL	2.2
49	D0	78	TYR	2.2
39	DQ	66	ILE	2.2
10	AJ	36	GLY	2.2
29	DC	219	GLY	2.2
39	DQ	33	GLY	2.2
40	DR	7	GLY	2.2
44	DV	76	LYS	2.2
25	AY	54	U	2.2
27	BA	2109	U	2.2
47	DY	53	PRO	2.2
4	AD	9	CYS	2.2
4	CD	26	CYS	2.2
29	DC	38	ASP	2.2
1	CA	1225	A	2.2
28	DB	52	A	2.2
1	CA	1026	G	2.2
1	CA	1456	G	2.2
27	BA	1414	G	2.2
27	DA	1139	G	2.2
27	DA	1740	G	2.2
27	DA	2751	G	2.2
28	DB	33	G	2.2
58	D9	3	VAL	2.1
47	DY	55	TYR	2.1
27	BA	2178	C	2.1
9	CI	85	LEU	2.1
4	AD	151	LYS	2.1
35	DI	121	LYS	2.1
29	BC	158	ALA	2.1
3	AC	126	ARG	2.1
10	AJ	66	ARG	2.1
29	BC	210	ARG	2.1
51	B2	12	GLU	2.1
12	AL	45	PRO	2.1
35	BI	132	PRO	2.1
25	AY	31	U	2.1
39	DQ	102	VAL	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
47	DY	45	VAL	2.1
27	BA	2310	A	2.1
34	DH	164	TYR	2.1
47	BY	96	ILE	2.1
29	BC	209	LEU	2.1
34	DH	64	LEU	2.1
1	AA	1190	G	2.1
4	CD	168	ARG	2.1
27	BA	171	G	2.1
38	DP	68	GLN	2.1
47	BY	2	ARG	2.1
56	D7	49	ARG	2.1
27	BA	2803	C	2.1
28	DB	17	C	2.1
35	BI	111	PRO	2.1
4	AD	12	CYS	2.1
58	D9	12	ASP	2.1
36	DN	101	HIS	2.1
1	AA	1086	U	2.1
10	AJ	82	ILE	2.1
20	AT	13	LEU	2.1
27	DA	362	U	2.1
41	BS	101	LEU	2.1
41	DS	57	LYS	2.1
48	DZ	162	LEU	2.1
49	D0	5	LYS	2.1
50	B1	85	LEU	2.1
53	D4	77	THR	2.1
29	BC	213	TYR	2.1
55	D6	34	LEU	2.1
16	CP	18	ARG	2.1
40	BR	8	ARG	2.1
49	D0	41	ARG	2.1
39	DQ	12	GLN	2.1
1	AA	88	A	2.1
1	CA	1447	A	2.1
3	CC	2	GLY	2.1
9	AI	12	GLU	2.1
17	AQ	78	GLU	2.1
18	CR	83	GLU	2.1
28	DB	26	A	2.1
31	DE	62	PRO	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
39	DQ	15	GLY	2.1
41	DS	64	GLU	2.1
57	B8	28	GLY	2.1
1	CA	108	G	2.1
1	CA	727	G	2.1
1	CA	1190	G	2.1
7	CG	80	VAL	2.1
27	DA	11	G	2.1
27	DA	352	G	2.1
27	DA	2104	G	2.1
1	AA	1028	C	2.1
27	DA	1589	C	2.1
4	AD	22	LYS	2.1
47	DY	4	LYS	2.1
57	D8	15	LYS	2.1
15	CO	57	LEU	2.1
41	DS	18	ILE	2.1
48	DZ	145	ILE	2.1
55	B6	13	CYS	2.1
2	AB	137	ARG	2.1
15	AO	69	TYR	2.1
40	DR	35	THR	2.1
41	DS	92	TYR	2.1
33	DG	171	ALA	2.1
27	BA	2113	U	2.1
13	CM	112	GLY	2.1
43	DU	118	GLY	2.1
53	D4	79	GLY	2.1
29	BC	181	PRO	2.1
33	BG	80	PHE	2.1
34	BH	12	PRO	2.1
14	AN	18	VAL	2.1
19	AS	9	VAL	2.1
1	AA	975	A	2.1
27	BA	1048	A	2.1
39	DQ	89	ASN	2.1
49	D0	46	LYS	2.1
58	D9	15	LYS	2.1
2	CB	39	ILE	2.1
29	DC	129	ARG	2.1
32	DF	28	ILE	2.1
33	DG	140	ILE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
48	DZ	143	LEU	2.1
40	DR	3	HIS	2.1
14	AN	13	THR	2.1
1	CA	980	C	2.1
1	CA	1149	C	2.1
1	AA	1003	G	2.1
3	CC	187	ALA	2.1
7	AG	2	ALA	2.1
27	DA	897	C	2.1
27	DA	898	C	2.1
27	BA	2149	G	2.1
27	DA	977	G	2.1
29	BC	198	ALA	2.1
5	CE	85	GLY	2.1
13	AM	119	GLY	2.1
20	CT	69	GLY	2.1
2	AB	70	PHE	2.1
34	BH	168	PRO	2.1
35	DI	134	PRO	2.1
38	BP	52	GLU	2.1
1	AA	202	U	2.0
2	CB	132	LYS	2.0
34	DH	153	LYS	2.0
39	DQ	35	VAL	2.0
44	DV	84	LYS	2.0
53	D4	36	VAL	2.0
7	CG	5	ARG	2.0
30	DD	244	ARG	2.0
43	DU	59	ARG	2.0
51	D2	30	ARG	2.0
54	B5	58	LEU	2.0
55	D6	9	LEU	2.0
57	D8	46	ARG	2.0
31	DE	135	HIS	2.0
10	CJ	58	ASP	2.0
11	AK	25	TYR	2.0
27	DA	2135	A	2.0
28	DB	66	A	2.0
29	BC	93	TYR	2.0
29	DC	204	ALA	2.0
44	DV	81	TYR	2.0
3	CC	25	GLY	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
29	BC	169	GLY	2.0
29	DC	176	GLY	2.0
34	DH	142	GLY	2.0
41	DS	60	GLY	2.0
1	AA	1354	C	2.0
13	AM	31	LYS	2.0
14	CN	8	GLU	2.0
39	DQ	112	GLU	2.0
27	BA	2477	C	2.0
27	DA	527	C	2.0
27	DA	2205	C	2.0
32	DF	11	VAL	2.0
1	AA	1127	G	2.0
1	CA	98	G	2.0
3	CC	179	ARG	2.0
27	DA	363	G	2.0
27	DA	614(B)	G	2.0
31	BE	61	ARG	2.0
38	BP	6	LEU	2.0
46	DX	60	ARG	2.0
29	DC	211	SER	2.0
1	CA	1257	U	2.0
27	BA	12	U	2.0
27	DA	2808	U	2.0
8	AH	1	MET	2.0
29	BC	57	ASN	2.0
13	AM	123	ALA	2.0
13	CM	75	ALA	2.0
29	BC	122	ALA	2.0
36	DN	4	TYR	2.0
38	DP	30	THR	2.0
38	BP	47	ASP	2.0
38	DP	22	GLY	2.0
13	AM	10	PRO	2.0
35	BI	119	PRO	2.0
2	CB	165	VAL	2.0
9	CI	16	ARG	2.0
10	AJ	5	ARG	2.0
14	CN	25	VAL	2.0
27	BA	1847	A	2.0
34	BH	159	GLU	2.0
37	DO	102	VAL	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
39	DQ	132	VAL	2.0
18	CR	85	LEU	2.0
33	DG	3	LEU	2.0
40	BR	10	LEU	2.0
30	DD	270	ILE	2.0
34	DH	121	ILE	2.0
1	AA	1145	C	2.0
23	CW	73	C	2.0
25	AY	55	C	2.0
27	DA	1505	C	2.0
27	DA	2306	C	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
26	UAL	CZ	3	9/10	0.81	0.15	91,92,93,93	0
26	KBE	CZ	1	9/10	0.82	0.23	95,98,100,100	0
26	UAL	AZ	3	9/10	0.85	0.12	63,66,70,71	0
26	DPP	AZ	5	6/7	0.85	0.15	62,64,65,65	0
26	DPP	CZ	2	6/7	0.87	0.12	92,93,95,98	0
26	KBE	AZ	1	9/10	0.87	0.19	71,74,78,79	0
26	MYN	CZ	4	11/12	0.91	0.12	88,89,91,92	0
26	DPP	CZ	5	6/7	0.92	0.14	88,89,89,90	0
26	MYN	AZ	4	11/12	0.93	0.12	61,64,65,65	0
26	DPP	AZ	2	6/7	0.93	0.12	66,67,69,71	0

5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	CA	1683	1/1	0.40	0.33	53,53,53,53	0
60	MG	CW	103	1/1	0.52	0.17	73,73,73,73	0
60	MG	DB	202	1/1	0.53	0.21	80,80,80,80	0
60	MG	DA	3190	1/1	0.54	0.20	43,43,43,43	0
60	MG	DA	3164	1/1	0.55	0.26	64,64,64,64	0
60	MG	CA	1611	1/1	0.56	0.36	66,66,66,66	0
60	MG	BA	3283	1/1	0.58	0.30	38,38,38,38	0
60	MG	CA	1696	1/1	0.60	0.19	91,91,91,91	0
60	MG	AA	1626	1/1	0.61	0.20	51,51,51,51	0
60	MG	CA	1652	1/1	0.62	0.26	61,61,61,61	0
60	MG	AA	1684	1/1	0.63	0.34	69,69,69,69	0
60	MG	DA	3027	1/1	0.64	0.34	38,38,38,38	0
60	MG	DA	3176	1/1	0.65	0.23	54,54,54,54	0
60	MG	DA	3053	1/1	0.65	0.28	32,32,32,32	0
60	MG	DA	3167	1/1	0.65	0.16	36,36,36,36	0
60	MG	CA	1633	1/1	0.66	0.19	62,62,62,62	0
60	MG	DA	3235	1/1	0.67	0.22	61,61,61,61	0
60	MG	AA	1640	1/1	0.67	0.14	70,70,70,70	0
60	MG	CA	1664	1/1	0.68	0.23	83,83,83,83	0
60	MG	BA	3195	1/1	0.68	0.35	49,49,49,49	0
60	MG	DA	3148	1/1	0.68	0.19	42,42,42,42	0
60	MG	DA	3128	1/1	0.69	0.28	24,24,24,24	0
60	MG	BA	3104	1/1	0.69	0.13	42,42,42,42	0
60	MG	DA	3162	1/1	0.69	0.26	44,44,44,44	0
60	MG	BA	3201	1/1	0.70	0.54	53,53,53,53	0
60	MG	AW	103	1/1	0.71	0.20	72,72,72,72	0
60	MG	DA	3231	1/1	0.71	0.30	49,49,49,49	0
60	MG	BA	3109	1/1	0.71	0.31	58,58,58,58	0
60	MG	DA	3122	1/1	0.71	0.19	40,40,40,40	0
60	MG	AA	1646	1/1	0.72	0.15	71,71,71,71	0
60	MG	AA	1637	1/1	0.72	0.19	44,44,44,44	0
60	MG	BA	3213	1/1	0.73	0.24	49,49,49,49	0
60	MG	BA	3190	1/1	0.73	0.15	39,39,39,39	0
60	MG	BA	3189	1/1	0.74	0.18	40,40,40,40	0
60	MG	DA	3188	1/1	0.74	0.21	72,72,72,72	0
60	MG	CA	1618	1/1	0.74	0.19	14,14,14,14	0
60	MG	AA	1702	1/1	0.74	0.23	41,41,41,41	0
60	MG	DA	3095	1/1	0.74	0.23	61,61,61,61	0
60	MG	CA	1641	1/1	0.74	0.33	66,66,66,66	0
60	MG	AA	1632	1/1	0.75	0.27	48,48,48,48	0
60	MG	BA	3162	1/1	0.75	0.23	56,56,56,56	0
60	MG	BA	3085	1/1	0.75	0.37	70,70,70,70	0
60	MG	AA	1681	1/1	0.75	0.14	58,58,58,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	CA	1647	1/1	0.75	0.34	44,44,44,44	0
60	MG	DA	3189	1/1	0.76	0.15	57,57,57,57	0
60	MG	AA	1630	1/1	0.77	0.42	62,62,62,62	0
60	MG	DA	3090	1/1	0.77	0.21	21,21,21,21	0
60	MG	BA	3313	1/1	0.77	0.29	45,45,45,45	0
60	MG	CA	1685	1/1	0.77	0.31	59,59,59,59	0
60	MG	BA	3328	1/1	0.78	0.20	34,34,34,34	0
60	MG	AA	1648	1/1	0.78	0.43	68,68,68,68	0
60	MG	DA	3175	1/1	0.78	0.32	72,72,72,72	0
60	MG	CA	1701	1/1	0.78	0.15	53,53,53,53	0
60	MG	AA	1638	1/1	0.78	0.40	76,76,76,76	0
60	MG	DF	301	1/1	0.78	0.14	53,53,53,53	0
60	MG	DA	3168	1/1	0.79	0.30	55,55,55,55	0
60	MG	DA	3227	1/1	0.79	0.19	36,36,36,36	0
60	MG	AX	103	1/1	0.79	0.19	51,51,51,51	0
60	MG	CA	1649	1/1	0.79	0.23	54,54,54,54	0
60	MG	BA	3289	1/1	0.79	0.26	42,42,42,42	0
60	MG	DA	3134	1/1	0.79	0.18	59,59,59,59	0
60	MG	AW	101	1/1	0.80	0.21	48,48,48,48	0
60	MG	BA	3164	1/1	0.80	0.19	33,33,33,33	0
60	MG	DA	3225	1/1	0.80	0.21	39,39,39,39	0
60	MG	AA	1644	1/1	0.80	0.33	39,39,39,39	0
60	MG	DA	3171	1/1	0.80	0.32	52,52,52,52	0
60	MG	DA	3138	1/1	0.80	0.25	63,63,63,63	0
60	MG	DA	3001	1/1	0.80	0.23	51,51,51,51	0
60	MG	DA	3117	1/1	0.80	0.27	49,49,49,49	0
60	MG	CA	1677	1/1	0.81	0.19	51,51,51,51	0
60	MG	AX	108	1/1	0.81	0.16	34,34,34,34	0
60	MG	BA	3050	1/1	0.81	0.27	1,1,1,1	0
60	MG	AA	1651	1/1	0.81	0.31	53,53,53,53	0
60	MG	CA	1644	1/1	0.81	0.47	67,67,67,67	0
60	MG	AA	1700	1/1	0.81	0.17	74,74,74,74	0
60	MG	DA	3144	1/1	0.81	0.25	53,53,53,53	0
60	MG	AA	1608	1/1	0.81	0.27	22,22,22,22	0
60	MG	BB	203	1/1	0.81	0.21	35,35,35,35	0
60	MG	BA	3144	1/1	0.81	0.32	59,59,59,59	0
60	MG	CA	1665	1/1	0.81	0.16	33,33,33,33	0
60	MG	DA	3091	1/1	0.81	0.25	55,55,55,55	0
60	MG	CA	1679	1/1	0.82	0.14	43,43,43,43	0
60	MG	BA	3329	1/1	0.82	0.18	45,45,45,45	0
60	MG	DA	3111	1/1	0.82	0.29	64,64,64,64	0
60	MG	CA	1645	1/1	0.82	0.36	56,56,56,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	BA	3281	1/1	0.82	0.18	21,21,21,21	0
60	MG	BA	3084	1/1	0.82	0.12	27,27,27,27	0
60	MG	DA	3131	1/1	0.82	0.46	63,63,63,63	0
60	MG	AX	104	1/1	0.82	0.11	57,57,57,57	0
60	MG	DA	3204	1/1	0.82	0.27	67,67,67,67	0
60	MG	DA	3221	1/1	0.82	0.28	52,52,52,52	0
60	MG	DA	3136	1/1	0.82	0.23	31,31,31,31	0
60	MG	CA	1624	1/1	0.82	0.32	40,40,40,40	0
60	MG	DA	3021	1/1	0.82	0.18	27,27,27,27	0
60	MG	AG	201	1/1	0.82	0.12	42,42,42,42	0
60	MG	CA	1675	1/1	0.82	0.31	31,31,31,31	0
60	MG	AA	1601	1/1	0.82	0.21	47,47,47,47	0
60	MG	DA	3115	1/1	0.83	0.22	36,36,36,36	0
60	MG	BA	3205	1/1	0.83	0.26	30,30,30,30	0
60	MG	AA	1704	1/1	0.83	0.22	13,13,13,13	0
60	MG	AA	1680	1/1	0.83	0.33	70,70,70,70	0
60	MG	AX	101	1/1	0.83	0.11	41,41,41,41	0
60	MG	DA	3237	1/1	0.83	0.20	10,10,10,10	0
60	MG	DA	3040	1/1	0.83	0.26	19,19,19,19	0
60	MG	DA	3114	1/1	0.83	0.11	34,34,34,34	0
60	MG	DA	3159	1/1	0.84	0.23	32,32,32,32	0
60	MG	AA	1643	1/1	0.84	0.14	29,29,29,29	0
60	MG	AA	1689	1/1	0.84	0.11	2,2,2,2	0
60	MG	AA	1690	1/1	0.84	0.23	23,23,23,23	0
60	MG	BA	3165	1/1	0.84	0.27	48,48,48,48	0
60	MG	AA	1705	1/1	0.84	0.11	4,4,4,4	0
60	MG	CA	1655	1/1	0.84	0.19	29,29,29,29	0
60	MG	CA	1638	1/1	0.84	0.25	31,31,31,31	0
60	MG	CA	1640	1/1	0.84	0.15	41,41,41,41	0
60	MG	BA	3222	1/1	0.84	0.16	26,26,26,26	0
60	MG	DO	201	1/1	0.84	0.08	65,65,65,65	0
60	MG	BA	3120	1/1	0.85	0.36	87,87,87,87	0
60	MG	DA	3181	1/1	0.85	0.20	50,50,50,50	0
60	MG	DA	3182	1/1	0.85	0.21	23,23,23,23	0
60	MG	BA	3204	1/1	0.85	0.29	25,25,25,25	0
60	MG	CA	1682	1/1	0.85	0.30	41,41,41,41	0
60	MG	BA	3167	1/1	0.85	0.21	22,22,22,22	0
60	MG	DA	3147	1/1	0.85	0.10	26,26,26,26	0
60	MG	B0	102	1/1	0.85	0.32	40,40,40,40	0
60	MG	BA	3186	1/1	0.85	0.21	60,60,60,60	0
60	MG	DA	3160	1/1	0.85	0.24	27,27,27,27	0
60	MG	BA	3187	1/1	0.85	0.16	17,17,17,17	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	AA	1671	1/1	0.85	0.12	49,49,49,49	0
60	MG	AA	1669	1/1	0.85	0.15	35,35,35,35	0
60	MG	DA	3239	1/1	0.85	0.11	34,34,34,34	0
60	MG	DA	3020	1/1	0.85	0.27	40,40,40,40	0
60	MG	BA	3191	1/1	0.85	0.16	6,6,6,6	0
60	MG	AA	1707	1/1	0.85	0.36	52,52,52,52	0
60	MG	CA	1609	1/1	0.86	0.20	50,50,50,50	0
60	MG	BA	3294	1/1	0.86	0.49	90,90,90,90	0
60	MG	DA	3008	1/1	0.86	0.24	13,13,13,13	0
60	MG	DA	3186	1/1	0.86	0.35	53,53,53,53	0
60	MG	CA	1616	1/1	0.86	0.32	52,52,52,52	0
60	MG	BA	3296	1/1	0.86	0.23	26,26,26,26	0
60	MG	BA	3059	1/1	0.86	0.15	25,25,25,25	0
60	MG	DA	3198	1/1	0.86	0.16	32,32,32,32	0
60	MG	DA	3200	1/1	0.86	0.21	42,42,42,42	0
60	MG	DA	3037	1/1	0.86	0.09	24,24,24,24	0
60	MG	CA	1670	1/1	0.86	0.19	26,26,26,26	0
60	MG	CA	1626	1/1	0.86	0.14	31,31,31,31	0
60	MG	BA	3159	1/1	0.86	0.20	20,20,20,20	0
60	MG	AA	1670	1/1	0.86	0.15	54,54,54,54	0
60	MG	BB	201	1/1	0.86	0.17	46,46,46,46	0
60	MG	BA	3117	1/1	0.86	0.30	1,1,1,1	0
60	MG	AA	1654	1/1	0.86	0.19	68,68,68,68	0
60	MG	CA	1603	1/1	0.86	0.19	38,38,38,38	0
60	MG	CA	1606	1/1	0.86	0.31	45,45,45,45	0
60	MG	DA	3121	1/1	0.86	0.19	34,34,34,34	0
60	MG	DA	3143	1/1	0.87	0.30	54,54,54,54	0
60	MG	CA	1694	1/1	0.87	0.43	51,51,51,51	0
60	MG	DA	3145	1/1	0.87	0.15	35,35,35,35	0
60	MG	BB	202	1/1	0.87	0.20	9,9,9,9	0
60	MG	BA	3270	1/1	0.87	0.23	32,32,32,32	0
60	MG	DA	3155	1/1	0.87	0.29	31,31,31,31	0
60	MG	BA	3297	1/1	0.87	0.20	42,42,42,42	0
60	MG	BA	3304	1/1	0.87	0.15	36,36,36,36	0
60	MG	DA	3005	1/1	0.87	0.27	28,28,28,28	0
60	MG	BA	3310	1/1	0.87	0.23	38,38,38,38	0
60	MG	AA	1696	1/1	0.87	0.23	20,20,20,20	0
60	MG	BA	3316	1/1	0.87	0.26	35,35,35,35	0
60	MG	AA	1618	1/1	0.87	0.31	22,22,22,22	0
60	MG	AA	1620	1/1	0.87	0.25	31,31,31,31	0
60	MG	AA	1708	1/1	0.87	0.23	41,41,41,41	0
60	MG	CA	1686	1/1	0.87	0.07	37,37,37,37	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	DA	3076	1/1	0.87	0.17	25,25,25,25	0
60	MG	DA	3098	1/1	0.88	0.17	27,27,27,27	0
60	MG	BA	3305	1/1	0.88	0.19	32,32,32,32	0
60	MG	CA	1607	1/1	0.88	0.27	29,29,29,29	0
60	MG	BA	3258	1/1	0.88	0.20	32,32,32,32	0
60	MG	BA	3158	1/1	0.88	0.32	35,35,35,35	0
60	MG	BA	3169	1/1	0.88	0.18	16,16,16,16	0
60	MG	BA	3171	1/1	0.88	0.15	36,36,36,36	0
60	MG	DA	3124	1/1	0.88	0.25	36,36,36,36	0
60	MG	BA	3001	1/1	0.88	0.27	43,43,43,43	0
60	MG	BA	3094	1/1	0.88	0.09	11,11,11,11	0
60	MG	CA	1629	1/1	0.88	0.19	16,16,16,16	0
60	MG	CA	1630	1/1	0.88	0.10	57,57,57,57	0
60	MG	AA	1683	1/1	0.88	0.14	16,16,16,16	0
60	MG	BA	3215	1/1	0.88	0.36	60,60,60,60	0
60	MG	DA	3213	1/1	0.88	0.25	31,31,31,31	0
60	MG	DA	3214	1/1	0.88	0.31	21,21,21,21	0
60	MG	DA	3217	1/1	0.88	0.16	27,27,27,27	0
60	MG	BA	3302	1/1	0.88	0.11	11,11,11,11	0
60	MG	DA	3063	1/1	0.88	0.20	24,24,24,24	0
60	MG	DA	3146	1/1	0.88	0.18	17,17,17,17	0
60	MG	CA	1684	1/1	0.88	0.13	33,33,33,33	0
60	MG	DA	3080	1/1	0.88	0.15	36,36,36,36	0
60	MG	DA	3084	1/1	0.88	0.22	71,71,71,71	0
60	MG	DA	3087	1/1	0.88	0.17	32,32,32,32	0
60	MG	CA	1602	1/1	0.88	0.23	26,26,26,26	0
60	MG	BA	3107	1/1	0.88	0.39	65,65,65,65	0
60	MG	CA	1692	1/1	0.88	0.23	32,32,32,32	0
60	MG	BA	3247	1/1	0.89	0.20	35,35,35,35	0
60	MG	BD	301	1/1	0.89	0.28	12,12,12,12	0
60	MG	BX	101	1/1	0.89	0.10	31,31,31,31	0
60	MG	DA	3048	1/1	0.89	0.18	23,23,23,23	0
60	MG	CA	1656	1/1	0.89	0.18	39,39,39,39	0
60	MG	BA	3033	1/1	0.89	0.29	1,1,1,1	0
60	MG	DA	3161	1/1	0.89	0.15	33,33,33,33	0
60	MG	DA	3075	1/1	0.89	0.29	1,1,1,1	0
60	MG	B0	103	1/1	0.89	0.18	22,22,22,22	0
60	MG	DA	3078	1/1	0.89	0.09	26,26,26,26	0
60	MG	BA	3036	1/1	0.89	0.27	8,8,8,8	0
60	MG	BA	3177	1/1	0.89	0.25	41,41,41,41	0
60	MG	DA	3086	1/1	0.89	0.33	58,58,58,58	0
60	MG	AA	1652	1/1	0.89	0.22	28,28,28,28	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	BA	3056	1/1	0.89	0.18	1,1,1,1	0
60	MG	BA	3291	1/1	0.89	0.22	14,14,14,14	0
60	MG	BA	3293	1/1	0.89	0.31	45,45,45,45	0
60	MG	BA	3122	1/1	0.89	0.19	12,12,12,12	0
60	MG	DA	3103	1/1	0.89	0.16	26,26,26,26	0
60	MG	DA	3104	1/1	0.89	0.26	42,42,42,42	0
60	MG	DA	3109	1/1	0.89	0.15	50,50,50,50	0
60	MG	BA	3128	1/1	0.89	0.19	16,16,16,16	0
60	MG	DA	3203	1/1	0.89	0.33	38,38,38,38	0
60	MG	AA	1613	1/1	0.89	0.17	36,36,36,36	0
60	MG	AA	1673	1/1	0.89	0.13	39,39,39,39	0
60	MG	AA	1603	1/1	0.89	0.13	32,32,32,32	0
60	MG	BA	3093	1/1	0.89	0.26	1,1,1,1	0
60	MG	CA	1700	1/1	0.89	0.22	36,36,36,36	0
60	MG	BA	3014	1/1	0.89	0.31	1,1,1,1	0
60	MG	CA	1702	1/1	0.89	0.18	27,27,27,27	0
60	MG	CW	101	1/1	0.89	0.06	55,55,55,55	0
60	MG	DA	3234	1/1	0.89	0.20	40,40,40,40	0
60	MG	BA	3210	1/1	0.89	0.28	33,33,33,33	0
60	MG	BA	3101	1/1	0.89	0.20	31,31,31,31	0
60	MG	BA	3029	1/1	0.89	0.21	36,36,36,36	0
60	MG	BA	3168	1/1	0.89	0.35	60,60,60,60	0
60	MG	BA	3238	1/1	0.89	0.22	29,29,29,29	0
60	MG	BA	3243	1/1	0.89	0.39	45,45,45,45	0
60	MG	D7	101	1/1	0.89	0.12	36,36,36,36	0
60	MG	AA	1605	1/1	0.90	0.09	35,35,35,35	0
60	MG	DA	3184	1/1	0.90	0.35	35,35,35,35	0
60	MG	DA	3185	1/1	0.90	0.13	10,10,10,10	0
60	MG	BA	3143	1/1	0.90	0.11	32,32,32,32	0
60	MG	DA	3141	1/1	0.90	0.20	36,36,36,36	0
60	MG	AA	1642	1/1	0.90	0.20	41,41,41,41	0
60	MG	DA	3009	1/1	0.90	0.17	12,12,12,12	0
60	MG	DA	3013	1/1	0.90	0.16	30,30,30,30	0
60	MG	BA	3237	1/1	0.90	0.18	1,1,1,1	0
60	MG	BA	3096	1/1	0.90	0.25	34,34,34,34	0
60	MG	AA	1647	1/1	0.90	0.20	39,39,39,39	0
60	MG	DA	3211	1/1	0.90	0.14	23,23,23,23	0
60	MG	BA	3160	1/1	0.90	0.34	29,29,29,29	0
60	MG	DA	3156	1/1	0.90	0.09	47,47,47,47	0
60	MG	DA	3216	1/1	0.90	0.14	24,24,24,24	0
60	MG	CA	1690	1/1	0.90	0.19	31,31,31,31	0
60	MG	DA	3218	1/1	0.90	0.31	50,50,50,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	DA	3042	1/1	0.90	0.12	46,46,46,46	0
60	MG	BA	3051	1/1	0.90	0.24	14,14,14,14	0
60	MG	DA	3116	1/1	0.90	0.27	47,47,47,47	0
60	MG	BA	3259	1/1	0.90	0.31	16,16,16,16	0
60	MG	DA	3166	1/1	0.90	0.28	36,36,36,36	0
60	MG	AA	1692	1/1	0.90	0.17	19,19,19,19	0
60	MG	BA	3200	1/1	0.90	0.22	14,14,14,14	0
60	MG	AA	1656	1/1	0.90	0.20	10,10,10,10	0
60	MG	AA	1665	1/1	0.90	0.13	31,31,31,31	0
60	MG	AA	1610	1/1	0.90	0.17	36,36,36,36	0
60	MG	DA	3177	1/1	0.90	0.12	13,13,13,13	0
60	MG	BA	3091	1/1	0.90	0.20	1,1,1,1	0
60	MG	BA	3211	1/1	0.91	0.38	36,36,36,36	0
60	MG	AA	1713	1/1	0.91	0.15	43,43,43,43	0
60	MG	DA	3178	1/1	0.91	0.13	22,22,22,22	0
60	MG	DA	3029	1/1	0.91	0.17	1,1,1,1	0
60	MG	BA	3284	1/1	0.91	0.15	21,21,21,21	0
60	MG	CA	1631	1/1	0.91	0.07	19,19,19,19	0
60	MG	AA	1685	1/1	0.91	0.24	69,69,69,69	0
60	MG	AA	1657	1/1	0.91	0.21	37,37,37,37	0
60	MG	BA	3229	1/1	0.91	0.26	49,49,49,49	0
60	MG	DA	3054	1/1	0.91	0.11	21,21,21,21	0
60	MG	BA	3194	1/1	0.91	0.37	54,54,54,54	0
60	MG	DA	3065	1/1	0.91	0.15	28,28,28,28	0
60	MG	DA	3199	1/1	0.91	0.15	35,35,35,35	0
60	MG	AA	1604	1/1	0.91	0.17	14,14,14,14	0
60	MG	DA	3201	1/1	0.91	0.19	36,36,36,36	0
60	MG	CA	1695	1/1	0.91	0.18	40,40,40,40	0
60	MG	BA	3240	1/1	0.91	0.40	75,75,75,75	0
60	MG	DA	3079	1/1	0.91	0.20	19,19,19,19	0
60	MG	AA	1678	1/1	0.91	0.25	29,29,29,29	0
60	MG	BA	3303	1/1	0.91	0.26	32,32,32,32	0
60	MG	AA	1679	1/1	0.91	0.13	36,36,36,36	0
60	MG	CA	1608	1/1	0.91	0.14	24,24,24,24	0
60	MG	DA	3157	1/1	0.91	0.30	58,58,58,58	0
60	MG	BA	3251	1/1	0.91	0.23	1,1,1,1	0
60	MG	DA	3222	1/1	0.91	0.12	24,24,24,24	0
60	MG	CW	104	1/1	0.91	0.11	57,57,57,57	0
60	MG	BA	3114	1/1	0.91	0.14	14,14,14,14	0
60	MG	DA	3003	1/1	0.91	0.14	17,17,17,17	0
60	MG	BA	3115	1/1	0.91	0.21	1,1,1,1	0
60	MG	CA	1617	1/1	0.91	0.18	1,1,1,1	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	CA	1672	1/1	0.91	0.18	21,21,21,21	0
60	MG	AA	1699	1/1	0.91	0.07	21,21,21,21	0
60	MG	DA	3170	1/1	0.91	0.19	33,33,33,33	0
60	MG	DA	3016	1/1	0.91	0.16	12,12,12,12	0
60	MG	DA	3174	1/1	0.91	0.22	6,6,6,6	0
60	MG	BA	3276	1/1	0.91	0.21	16,16,16,16	0
60	MG	DA	3154	1/1	0.92	0.13	38,38,38,38	0
60	MG	DA	3049	1/1	0.92	0.21	36,36,36,36	0
60	MG	CA	1673	1/1	0.92	0.10	15,15,15,15	0
60	MG	BA	3108	1/1	0.92	0.24	2,2,2,2	0
60	MG	DA	3158	1/1	0.92	0.15	49,49,49,49	0
60	MG	DA	3059	1/1	0.92	0.20	6,6,6,6	0
60	MG	BA	3064	1/1	0.92	0.32	45,45,45,45	0
60	MG	DA	3064	1/1	0.92	0.15	12,12,12,12	0
60	MG	BA	3077	1/1	0.92	0.20	1,1,1,1	0
60	MG	DA	3073	1/1	0.92	0.20	58,58,58,58	0
60	MG	BA	3026	1/1	0.92	0.19	7,7,7,7	0
60	MG	BA	3027	1/1	0.92	0.28	1,1,1,1	0
60	MG	AA	1664	1/1	0.92	0.19	46,46,46,46	0
60	MG	BA	3223	1/1	0.92	0.32	42,42,42,42	0
60	MG	BA	3226	1/1	0.92	0.23	39,39,39,39	0
60	MG	CA	1619	1/1	0.92	0.24	20,20,20,20	0
60	MG	CA	1691	1/1	0.92	0.11	21,21,21,21	0
60	MG	CA	1621	1/1	0.92	0.20	30,30,30,30	0
60	MG	DA	3088	1/1	0.92	0.21	22,22,22,22	0
60	MG	AA	1661	1/1	0.92	0.13	21,21,21,21	0
60	MG	BA	3173	1/1	0.92	0.20	50,50,50,50	0
60	MG	AW	102	1/1	0.92	0.07	36,36,36,36	0
60	MG	DA	3096	1/1	0.92	0.14	16,16,16,16	0
60	MG	BA	3133	1/1	0.92	0.24	1,1,1,1	0
60	MG	BA	3312	1/1	0.92	0.16	22,22,22,22	0
60	MG	BA	3241	1/1	0.92	0.53	80,80,80,80	0
60	MG	DA	3107	1/1	0.92	0.15	37,37,37,37	0
60	MG	BA	3140	1/1	0.92	0.35	26,26,26,26	0
60	MG	CA	1639	1/1	0.92	0.18	16,16,16,16	0
60	MG	BA	3141	1/1	0.92	0.21	17,17,17,17	0
60	MG	BA	3250	1/1	0.92	0.11	12,12,12,12	0
60	MG	CA	1643	1/1	0.92	0.14	7,7,7,7	0
60	MG	BA	3330	1/1	0.92	0.10	12,12,12,12	0
60	MG	AA	1709	1/1	0.92	0.16	36,36,36,36	0
60	MG	BA	3097	1/1	0.92	0.27	44,44,44,44	0
60	MG	DA	3123	1/1	0.92	0.30	40,40,40,40	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	BA	3149	1/1	0.92	0.12	14,14,14,14	0
60	MG	DA	3127	1/1	0.92	0.14	20,20,20,20	0
60	MG	BA	3266	1/1	0.92	0.21	12,12,12,12	0
60	MG	DA	3129	1/1	0.92	0.09	20,20,20,20	0
60	MG	BE	302	1/1	0.92	0.19	1,1,1,1	0
60	MG	BA	3151	1/1	0.92	0.17	22,22,22,22	0
60	MG	DA	3026	1/1	0.92	0.14	4,4,4,4	0
60	MG	CA	1662	1/1	0.92	0.15	38,38,38,38	0
60	MG	DA	3228	1/1	0.92	0.21	34,34,34,34	0
60	MG	BA	3274	1/1	0.92	0.14	21,21,21,21	0
60	MG	DA	3142	1/1	0.92	0.05	37,37,37,37	0
60	MG	AA	1682	1/1	0.92	0.12	48,48,48,48	0
60	MG	DA	3039	1/1	0.92	0.10	53,53,53,53	0
60	MG	CA	1668	1/1	0.92	0.19	30,30,30,30	0
60	MG	DB	201	1/1	0.92	0.18	51,51,51,51	0
60	MG	BA	3021	1/1	0.92	0.21	1,1,1,1	0
60	MG	DA	3047	1/1	0.92	0.20	29,29,29,29	0
60	MG	BA	3022	1/1	0.92	0.23	19,19,19,19	0
60	MG	DA	3153	1/1	0.92	0.13	13,13,13,13	0
60	MG	CA	1676	1/1	0.93	0.06	25,25,25,25	0
60	MG	CA	1612	1/1	0.93	0.37	35,35,35,35	0
60	MG	DA	3055	1/1	0.93	0.15	17,17,17,17	0
60	MG	DA	3057	1/1	0.93	0.07	32,32,32,32	0
60	MG	CA	1613	1/1	0.93	0.32	36,36,36,36	0
60	MG	DA	3060	1/1	0.93	0.16	23,23,23,23	0
60	MG	CA	1680	1/1	0.93	0.07	44,44,44,44	0
60	MG	BA	3230	1/1	0.93	0.14	19,19,19,19	0
60	MG	BA	3301	1/1	0.93	0.15	16,16,16,16	0
60	MG	DA	3071	1/1	0.93	0.13	19,19,19,19	0
60	MG	DA	3072	1/1	0.93	0.10	8,8,8,8	0
60	MG	BA	3135	1/1	0.93	0.15	20,20,20,20	0
60	MG	AX	106	1/1	0.93	0.26	25,25,25,25	0
60	MG	AA	1691	1/1	0.93	0.28	23,23,23,23	0
60	MG	CA	1688	1/1	0.93	0.11	37,37,37,37	0
60	MG	AA	1633	1/1	0.93	0.13	8,8,8,8	0
60	MG	DA	3172	1/1	0.93	0.18	6,6,6,6	0
60	MG	BA	3003	1/1	0.93	0.21	64,64,64,64	0
60	MG	BA	3245	1/1	0.93	0.14	25,25,25,25	0
60	MG	BA	3147	1/1	0.93	0.13	8,8,8,8	0
60	MG	BA	3249	1/1	0.93	0.34	13,13,13,13	0
60	MG	CA	1632	1/1	0.93	0.14	6,6,6,6	0
60	MG	CA	1698	1/1	0.93	0.18	29,29,29,29	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	CA	1699	1/1	0.93	0.09	30,30,30,30	0
60	MG	DA	3094	1/1	0.93	0.16	16,16,16,16	0
60	MG	BA	3320	1/1	0.93	0.12	23,23,23,23	0
60	MG	CA	1636	1/1	0.93	0.24	26,26,26,26	0
60	MG	CA	1637	1/1	0.93	0.54	57,57,57,57	0
60	MG	CE	201	1/1	0.93	0.12	56,56,56,56	0
60	MG	BA	3325	1/1	0.93	0.10	19,19,19,19	0
60	MG	BA	3004	1/1	0.93	0.18	8,8,8,8	0
60	MG	BA	3053	1/1	0.93	0.20	1,1,1,1	0
60	MG	BA	3197	1/1	0.93	0.16	24,24,24,24	0
60	MG	BA	3106	1/1	0.93	0.15	3,3,3,3	0
60	MG	BA	3263	1/1	0.93	0.29	47,47,47,47	0
60	MG	BA	3006	1/1	0.93	0.31	37,37,37,37	0
60	MG	BA	3203	1/1	0.93	0.17	17,17,17,17	0
60	MG	BA	3007	1/1	0.93	0.25	1,1,1,1	0
60	MG	BG	201	1/1	0.93	0.14	30,30,30,30	0
60	MG	DA	3215	1/1	0.93	0.15	23,23,23,23	0
60	MG	AA	1659	1/1	0.93	0.13	23,23,23,23	0
60	MG	AA	1686	1/1	0.93	0.36	34,34,34,34	0
60	MG	DA	3025	1/1	0.93	0.18	1,1,1,1	0
60	MG	CA	1660	1/1	0.93	0.13	21,21,21,21	0
60	MG	BA	3079	1/1	0.93	0.13	7,7,7,7	0
60	MG	CA	1663	1/1	0.93	0.05	31,31,31,31	0
60	MG	DA	3035	1/1	0.93	0.20	1,1,1,1	0
60	MG	BA	3080	1/1	0.93	0.22	15,15,15,15	0
60	MG	DA	3229	1/1	0.93	0.12	20,20,20,20	0
60	MG	BA	3287	1/1	0.93	0.09	7,7,7,7	0
60	MG	BA	3082	1/1	0.93	0.22	44,44,44,44	0
60	MG	AA	1660	1/1	0.93	0.28	49,49,49,49	0
60	MG	DA	3043	1/1	0.93	0.15	9,9,9,9	0
60	MG	DA	3046	1/1	0.93	0.11	28,28,28,28	0
60	MG	AA	1710	1/1	0.93	0.31	29,29,29,29	0
60	MG	BA	3172	1/1	0.93	0.11	18,18,18,18	0
60	MG	DD	301	1/1	0.93	0.13	21,21,21,21	0
60	MG	AA	1625	1/1	0.93	0.15	21,21,21,21	0
60	MG	DA	3052	1/1	0.93	0.17	14,14,14,14	0
60	MG	DA	3149	1/1	0.93	0.22	39,39,39,39	0
60	MG	BA	3046	1/1	0.94	0.18	10,10,10,10	0
60	MG	DA	3036	1/1	0.94	0.10	5,5,5,5	0
60	MG	AA	1619	1/1	0.94	0.04	10,10,10,10	0
60	MG	BA	3236	1/1	0.94	0.21	11,11,11,11	0
60	MG	BA	3314	1/1	0.94	0.11	35,35,35,35	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	BA	3008	1/1	0.94	0.09	4,4,4,4	0
60	MG	CA	1653	1/1	0.94	0.18	36,36,36,36	0
60	MG	BA	3010	1/1	0.94	0.20	2,2,2,2	0
60	MG	AA	1677	1/1	0.94	0.19	30,30,30,30	0
60	MG	BA	3326	1/1	0.94	0.17	21,21,21,21	0
60	MG	BA	3016	1/1	0.94	0.16	1,1,1,1	0
60	MG	BA	3062	1/1	0.94	0.21	1,1,1,1	0
60	MG	BA	3018	1/1	0.94	0.19	1,1,1,1	0
60	MG	BA	3332	1/1	0.94	0.22	1,1,1,1	0
60	MG	BA	3334	1/1	0.94	0.12	1,1,1,1	0
60	MG	BA	3174	1/1	0.94	0.05	7,7,7,7	0
60	MG	BA	3248	1/1	0.94	0.21	34,34,34,34	0
60	MG	BA	3176	1/1	0.94	0.14	1,1,1,1	0
60	MG	BB	204	1/1	0.94	0.14	21,21,21,21	0
60	MG	BA	3116	1/1	0.94	0.19	26,26,26,26	0
60	MG	BA	3184	1/1	0.94	0.29	40,40,40,40	0
60	MG	DA	3066	1/1	0.94	0.28	40,40,40,40	0
60	MG	BA	3256	1/1	0.94	0.20	23,23,23,23	0
60	MG	BU	201	1/1	0.94	0.18	23,23,23,23	0
60	MG	BA	3069	1/1	0.94	0.18	1,1,1,1	0
60	MG	BA	3073	1/1	0.94	0.19	1,1,1,1	0
60	MG	BA	3261	1/1	0.94	0.15	16,16,16,16	0
60	MG	BA	3074	1/1	0.94	0.17	4,4,4,4	0
60	MG	BA	3264	1/1	0.94	0.32	32,32,32,32	0
60	MG	BA	3127	1/1	0.94	0.17	1,1,1,1	0
60	MG	BA	3075	1/1	0.94	0.12	2,2,2,2	0
60	MG	BA	3193	1/1	0.94	0.29	22,22,22,22	0
60	MG	AA	1712	1/1	0.94	0.29	36,36,36,36	0
60	MG	CA	1693	1/1	0.94	0.10	20,20,20,20	0
60	MG	CA	1610	1/1	0.94	0.13	48,48,48,48	0
60	MG	BA	3279	1/1	0.94	0.15	29,29,29,29	0
60	MG	BA	3078	1/1	0.94	0.22	1,1,1,1	0
60	MG	DA	3191	1/1	0.94	0.21	31,31,31,31	0
60	MG	DA	3195	1/1	0.94	0.17	18,18,18,18	0
60	MG	CA	1697	1/1	0.94	0.14	27,27,27,27	0
60	MG	BA	3282	1/1	0.94	0.17	20,20,20,20	0
60	MG	DA	3097	1/1	0.94	0.07	51,51,51,51	0
60	MG	CA	1614	1/1	0.94	0.37	50,50,50,50	0
60	MG	DA	3100	1/1	0.94	0.12	18,18,18,18	0
60	MG	AA	1703	1/1	0.94	0.18	35,35,35,35	0
60	MG	DA	3205	1/1	0.94	0.09	2,2,2,2	0
60	MG	AA	1649	1/1	0.94	0.10	25,25,25,25	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	BA	3285	1/1	0.94	0.13	1,1,1,1	0
60	MG	BA	3142	1/1	0.94	0.06	30,30,30,30	0
60	MG	DA	3110	1/1	0.94	0.13	48,48,48,48	0
60	MG	CV	601	1/1	0.94	0.22	16,16,16,16	0
60	MG	BA	3202	1/1	0.94	0.13	1,1,1,1	0
60	MG	CW	102	1/1	0.94	0.07	40,40,40,40	0
60	MG	DA	3219	1/1	0.94	0.06	19,19,19,19	0
60	MG	DA	3220	1/1	0.94	0.25	30,30,30,30	0
60	MG	CA	1623	1/1	0.94	0.26	33,33,33,33	0
60	MG	AA	1695	1/1	0.94	0.16	30,30,30,30	0
60	MG	BA	3292	1/1	0.94	0.19	27,27,27,27	0
60	MG	AA	1687	1/1	0.94	0.17	20,20,20,20	0
60	MG	BA	3146	1/1	0.94	0.09	13,13,13,13	0
60	MG	BA	3295	1/1	0.94	0.14	41,41,41,41	0
60	MG	DA	3125	1/1	0.94	0.06	49,49,49,49	0
60	MG	AA	1645	1/1	0.94	0.17	22,22,22,22	0
60	MG	AW	104	1/1	0.94	0.15	31,31,31,31	0
60	MG	BA	3300	1/1	0.94	0.14	22,22,22,22	0
60	MG	DA	3238	1/1	0.94	0.39	42,42,42,42	0
60	MG	DA	3130	1/1	0.94	0.07	27,27,27,27	0
60	MG	BA	3092	1/1	0.94	0.20	3,3,3,3	0
60	MG	BA	3037	1/1	0.94	0.24	33,33,33,33	0
60	MG	DB	203	1/1	0.94	0.05	54,54,54,54	0
60	MG	BA	3041	1/1	0.94	0.20	1,1,1,1	0
60	MG	BA	3042	1/1	0.94	0.06	1,1,1,1	0
60	MG	BA	3043	1/1	0.94	0.23	1,1,1,1	0
60	MG	BA	3309	1/1	0.94	0.08	1,1,1,1	0
61	ZN	B5	102	1/1	0.94	0.07	51,51,51,51	0
60	MG	DA	3069	1/1	0.95	0.17	6,6,6,6	0
60	MG	AA	1672	1/1	0.95	0.12	53,53,53,53	0
60	MG	BA	3040	1/1	0.95	0.22	1,1,1,1	0
60	MG	BA	3005	1/1	0.95	0.35	1,1,1,1	0
60	MG	BA	3322	1/1	0.95	0.16	10,10,10,10	0
60	MG	BA	3260	1/1	0.95	0.57	65,65,65,65	0
60	MG	BA	3132	1/1	0.95	0.18	1,1,1,1	0
60	MG	AA	1706	1/1	0.95	0.08	28,28,28,28	0
60	MG	AA	1629	1/1	0.95	0.31	51,51,51,51	0
60	MG	DA	3082	1/1	0.95	0.13	15,15,15,15	0
60	MG	DA	3083	1/1	0.95	0.39	35,35,35,35	0
60	MG	BA	3212	1/1	0.95	0.12	11,11,11,11	0
60	MG	BA	3044	1/1	0.95	0.20	1,1,1,1	0
60	MG	BA	3271	1/1	0.95	0.18	28,28,28,28	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	CA	1642	1/1	0.95	0.10	28,28,28,28	0
60	MG	BA	3076	1/1	0.95	0.19	1,1,1,1	0
60	MG	BA	3217	1/1	0.95	0.05	1,1,1,1	0
60	MG	DA	3093	1/1	0.95	0.22	31,31,31,31	0
60	MG	AX	109	1/1	0.95	0.06	16,16,16,16	0
60	MG	BA	3105	1/1	0.95	0.09	8,8,8,8	0
60	MG	CA	1648	1/1	0.95	0.13	24,24,24,24	0
60	MG	BA	3224	1/1	0.95	0.11	20,20,20,20	0
60	MG	BA	3225	1/1	0.95	0.13	9,9,9,9	0
60	MG	BE	303	1/1	0.95	0.25	58,58,58,58	0
60	MG	CA	1654	1/1	0.95	0.08	44,44,44,44	0
60	MG	BA	3178	1/1	0.95	0.19	1,1,1,1	0
60	MG	DA	3018	1/1	0.95	0.09	15,15,15,15	0
60	MG	BA	3227	1/1	0.95	0.13	33,33,33,33	0
60	MG	CA	1658	1/1	0.95	0.25	30,30,30,30	0
60	MG	DA	3024	1/1	0.95	0.11	5,5,5,5	0
60	MG	DA	3112	1/1	0.95	0.17	7,7,7,7	0
60	MG	BA	3286	1/1	0.95	0.24	18,18,18,18	0
60	MG	DA	3202	1/1	0.95	0.13	18,18,18,18	0
60	MG	B0	101	1/1	0.95	0.18	4,4,4,4	0
60	MG	BA	3228	1/1	0.95	0.21	52,52,52,52	0
60	MG	BA	3009	1/1	0.95	0.21	1,1,1,1	0
60	MG	DA	3209	1/1	0.95	0.12	5,5,5,5	0
60	MG	DA	3118	1/1	0.95	0.28	22,22,22,22	0
60	MG	DA	3119	1/1	0.95	0.15	5,5,5,5	0
60	MG	DA	3120	1/1	0.95	0.17	3,3,3,3	0
60	MG	AA	1628	1/1	0.95	0.14	10,10,10,10	0
60	MG	BA	3232	1/1	0.95	0.17	1,1,1,1	0
60	MG	BA	3234	1/1	0.95	0.12	15,15,15,15	0
60	MG	DA	3038	1/1	0.95	0.13	8,8,8,8	0
60	MG	BA	3013	1/1	0.95	0.18	1,1,1,1	0
60	MG	BA	3188	1/1	0.95	0.18	30,30,30,30	0
60	MG	DA	3041	1/1	0.95	0.22	1,1,1,1	0
60	MG	CA	1674	1/1	0.95	0.25	55,55,55,55	0
60	MG	DA	3223	1/1	0.95	0.10	13,13,13,13	0
60	MG	BA	3034	1/1	0.95	0.25	1,1,1,1	0
60	MG	BA	3110	1/1	0.95	0.23	6,6,6,6	0
60	MG	BA	3152	1/1	0.95	0.17	6,6,6,6	0
60	MG	BA	3242	1/1	0.95	0.28	49,49,49,49	0
60	MG	BA	3155	1/1	0.95	0.14	14,14,14,14	0
60	MG	DA	3051	1/1	0.95	0.12	18,18,18,18	0
60	MG	BA	3244	1/1	0.95	0.22	34,34,34,34	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	BA	3083	1/1	0.95	0.24	1,1,1,1	0
60	MG	BA	3057	1/1	0.95	0.11	3,3,3,3	0
60	MG	BA	3308	1/1	0.95	0.18	30,30,30,30	0
60	MG	AA	1636	1/1	0.95	0.20	28,28,28,28	0
60	MG	CA	1687	1/1	0.95	0.17	17,17,17,17	0
60	MG	BA	3198	1/1	0.95	0.11	5,5,5,5	0
60	MG	BA	3311	1/1	0.95	0.30	40,40,40,40	0
60	MG	BA	3088	1/1	0.95	0.13	1,1,1,1	0
60	MG	CA	1625	1/1	0.95	0.15	3,3,3,3	0
60	MG	BA	3089	1/1	0.95	0.12	12,12,12,12	0
60	MG	DA	3067	1/1	0.95	0.13	23,23,23,23	0
60	MG	CA	1657	1/1	0.96	0.27	23,23,23,23	0
60	MG	BA	3333	1/1	0.96	0.21	1,1,1,1	0
60	MG	BA	3253	1/1	0.96	0.23	39,39,39,39	0
60	MG	BA	3025	1/1	0.96	0.27	31,31,31,31	0
60	MG	BA	3192	1/1	0.96	0.26	31,31,31,31	0
60	MG	DA	3050	1/1	0.96	0.06	38,38,38,38	0
60	MG	BA	3139	1/1	0.96	0.14	1,1,1,1	0
60	MG	BA	3086	1/1	0.96	0.11	4,4,4,4	0
60	MG	AA	1614	1/1	0.96	0.09	22,22,22,22	0
60	MG	DA	3150	1/1	0.96	0.08	28,28,28,28	0
60	MG	DA	3152	1/1	0.96	0.17	8,8,8,8	0
60	MG	BA	3196	1/1	0.96	0.12	21,21,21,21	0
60	MG	BA	3054	1/1	0.96	0.09	6,6,6,6	0
60	MG	AA	1617	1/1	0.96	0.09	13,13,13,13	0
60	MG	BA	3267	1/1	0.96	0.09	6,6,6,6	0
60	MG	BU	202	1/1	0.96	0.19	1,1,1,1	0
60	MG	DA	3062	1/1	0.96	0.12	8,8,8,8	0
60	MG	BA	3269	1/1	0.96	0.24	12,12,12,12	0
60	MG	AA	1663	1/1	0.96	0.27	14,14,14,14	0
60	MG	BA	3145	1/1	0.96	0.12	31,31,31,31	0
60	MG	BA	3058	1/1	0.96	0.12	1,1,1,1	0
60	MG	DA	3163	1/1	0.96	0.23	32,32,32,32	0
60	MG	CA	1681	1/1	0.96	0.27	44,44,44,44	0
60	MG	DA	3068	1/1	0.96	0.06	9,9,9,9	0
60	MG	B5	101	1/1	0.96	0.08	16,16,16,16	0
60	MG	CA	1601	1/1	0.96	0.21	1,1,1,1	0
60	MG	BA	3032	1/1	0.96	0.16	1,1,1,1	0
60	MG	BA	3278	1/1	0.96	0.07	15,15,15,15	0
60	MG	BA	3061	1/1	0.96	0.12	17,17,17,17	0
60	MG	DA	3173	1/1	0.96	0.09	10,10,10,10	0
60	MG	AA	1674	1/1	0.96	0.11	32,32,32,32	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	BA	3207	1/1	0.96	0.21	21,21,21,21	0
60	MG	AX	102	1/1	0.96	0.13	57,57,57,57	0
60	MG	BA	3102	1/1	0.96	0.12	1,1,1,1	0
60	MG	BA	3157	1/1	0.96	0.17	10,10,10,10	0
60	MG	DA	3180	1/1	0.96	0.21	5,5,5,5	0
60	MG	BA	3065	1/1	0.96	0.13	2,2,2,2	0
60	MG	BA	3066	1/1	0.96	0.09	1,1,1,1	0
60	MG	BA	3216	1/1	0.96	0.13	25,25,25,25	0
60	MG	CA	1615	1/1	0.96	0.20	28,28,28,28	0
60	MG	BA	3068	1/1	0.96	0.06	11,11,11,11	0
60	MG	DA	3187	1/1	0.96	0.04	27,27,27,27	0
60	MG	BA	3219	1/1	0.96	0.05	15,15,15,15	0
60	MG	BA	3221	1/1	0.96	0.28	35,35,35,35	0
60	MG	DA	3092	1/1	0.96	0.05	17,17,17,17	0
60	MG	BA	3161	1/1	0.96	0.29	24,24,24,24	0
60	MG	DA	3192	1/1	0.96	0.15	10,10,10,10	0
60	MG	DA	3193	1/1	0.96	0.12	29,29,29,29	0
60	MG	DA	3194	1/1	0.96	0.27	44,44,44,44	0
60	MG	AA	1621	1/1	0.96	0.23	28,28,28,28	0
60	MG	DA	3196	1/1	0.96	0.16	1,1,1,1	0
60	MG	BA	3163	1/1	0.96	0.07	12,12,12,12	0
60	MG	BA	3071	1/1	0.96	0.16	1,1,1,1	0
60	MG	BA	3299	1/1	0.96	0.10	13,13,13,13	0
60	MG	BA	3072	1/1	0.96	0.07	6,6,6,6	0
60	MG	DA	3099	1/1	0.96	0.05	14,14,14,14	0
60	MG	CA	1628	1/1	0.96	0.08	12,12,12,12	0
60	MG	BA	3166	1/1	0.96	0.16	8,8,8,8	0
60	MG	AA	1697	1/1	0.96	0.06	27,27,27,27	0
60	MG	DA	3207	1/1	0.96	0.12	1,1,1,1	0
60	MG	DA	3105	1/1	0.96	0.11	59,59,59,59	0
60	MG	BA	3112	1/1	0.96	0.06	11,11,11,11	0
60	MG	DA	3212	1/1	0.96	0.05	4,4,4,4	0
60	MG	DA	3002	1/1	0.96	0.11	9,9,9,9	0
60	MG	BA	3113	1/1	0.96	0.14	1,1,1,1	0
60	MG	BA	3170	1/1	0.96	0.32	55,55,55,55	0
60	MG	CA	1634	1/1	0.96	0.14	16,16,16,16	0
60	MG	DA	3113	1/1	0.96	0.18	2,2,2,2	0
60	MG	BA	3039	1/1	0.96	0.20	1,1,1,1	0
60	MG	BA	3235	1/1	0.96	0.13	1,1,1,1	0
60	MG	AA	1698	1/1	0.96	0.09	23,23,23,23	0
60	MG	AA	1612	1/1	0.96	0.13	15,15,15,15	0
60	MG	AA	1658	1/1	0.96	0.10	1,1,1,1	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	BA	3119	1/1	0.96	0.14	91,91,91,91	0
60	MG	BA	3017	1/1	0.96	0.18	1,1,1,1	0
60	MG	DA	3226	1/1	0.96	0.06	30,30,30,30	0
60	MG	AA	1688	1/1	0.96	0.06	49,49,49,49	0
60	MG	BA	3319	1/1	0.96	0.15	31,31,31,31	0
60	MG	BA	3179	1/1	0.96	0.10	17,17,17,17	0
60	MG	DA	3028	1/1	0.96	0.16	1,1,1,1	0
60	MG	BA	3180	1/1	0.96	0.14	40,40,40,40	0
60	MG	DA	3126	1/1	0.96	0.16	7,7,7,7	0
60	MG	BA	3323	1/1	0.96	0.15	2,2,2,2	0
60	MG	BA	3123	1/1	0.96	0.12	6,6,6,6	0
60	MG	CA	1651	1/1	0.96	0.35	35,35,35,35	0
60	MG	BA	3125	1/1	0.96	0.08	1,1,1,1	0
60	MG	BA	3002	1/1	0.96	0.24	17,17,17,17	0
60	MG	BA	3047	1/1	0.96	0.14	1,1,1,1	0
60	MG	BA	3049	1/1	0.96	0.14	1,1,1,1	0
60	MG	DD	302	1/1	0.96	0.17	6,6,6,6	0
60	MG	DA	3137	1/1	0.96	0.33	39,39,39,39	0
60	MG	AA	1631	1/1	0.96	0.25	12,12,12,12	0
60	MG	D0	101	1/1	0.96	0.19	12,12,12,12	0
60	MG	D5	101	1/1	0.96	0.10	10,10,10,10	0
60	MG	DA	3139	1/1	0.96	0.15	1,1,1,1	0
60	MG	DA	3140	1/1	0.96	0.12	24,24,24,24	0
60	MG	CA	1659	1/1	0.97	0.35	46,46,46,46	0
60	MG	CA	1604	1/1	0.97	0.19	1,1,1,1	0
60	MG	CA	1605	1/1	0.97	0.22	6,6,6,6	0
60	MG	DA	3101	1/1	0.97	0.19	20,20,20,20	0
60	MG	DA	3102	1/1	0.97	0.16	1,1,1,1	0
60	MG	BA	3100	1/1	0.97	0.06	10,10,10,10	0
60	MG	BA	3307	1/1	0.97	0.16	19,19,19,19	0
60	MG	BA	3060	1/1	0.97	0.13	4,4,4,4	0
60	MG	BA	3124	1/1	0.97	0.11	13,13,13,13	0
60	MG	DA	3033	1/1	0.97	0.10	4,4,4,4	0
60	MG	CA	1669	1/1	0.97	0.09	16,16,16,16	0
60	MG	BA	3265	1/1	0.97	0.13	13,13,13,13	0
60	MG	CA	1671	1/1	0.97	0.11	24,24,24,24	0
60	MG	AA	1701	1/1	0.97	0.11	11,11,11,11	0
60	MG	BA	3126	1/1	0.97	0.12	5,5,5,5	0
60	MG	BA	3268	1/1	0.97	0.13	1,1,1,1	0
60	MG	BA	3103	1/1	0.97	0.13	1,1,1,1	0
60	MG	BA	3315	1/1	0.97	0.21	29,29,29,29	0
60	MG	AA	1616	1/1	0.97	0.20	32,32,32,32	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	BA	3129	1/1	0.97	0.15	1,1,1,1	0
60	MG	BA	3272	1/1	0.97	0.22	15,15,15,15	0
60	MG	BA	3321	1/1	0.97	0.19	1,1,1,1	0
60	MG	BA	3231	1/1	0.97	0.12	2,2,2,2	0
60	MG	CA	1622	1/1	0.97	0.12	12,12,12,12	0
60	MG	DA	3197	1/1	0.97	0.17	21,21,21,21	0
60	MG	BA	3130	1/1	0.97	0.20	1,1,1,1	0
60	MG	BA	3031	1/1	0.97	0.21	1,1,1,1	0
60	MG	AA	1607	1/1	0.97	0.48	51,51,51,51	0
60	MG	BA	3327	1/1	0.97	0.17	17,17,17,17	0
60	MG	BA	3280	1/1	0.97	0.08	7,7,7,7	0
60	MG	BA	3134	1/1	0.97	0.18	12,12,12,12	0
60	MG	BA	3048	1/1	0.97	0.17	1,1,1,1	0
60	MG	BA	3331	1/1	0.97	0.28	35,35,35,35	0
60	MG	DA	3133	1/1	0.97	0.12	16,16,16,16	0
60	MG	BA	3136	1/1	0.97	0.32	42,42,42,42	0
60	MG	DA	3210	1/1	0.97	0.06	2,2,2,2	0
60	MG	DA	3135	1/1	0.97	0.13	11,11,11,11	0
60	MG	BA	3067	1/1	0.97	0.04	1,1,1,1	0
60	MG	AA	1653	1/1	0.97	0.14	38,38,38,38	0
60	MG	CA	1635	1/1	0.97	0.11	20,20,20,20	0
60	MG	AA	1622	1/1	0.97	0.15	12,12,12,12	0
60	MG	BA	3035	1/1	0.97	0.12	1,1,1,1	0
60	MG	BA	3288	1/1	0.97	0.16	29,29,29,29	0
60	MG	BA	3209	1/1	0.97	0.17	24,24,24,24	0
60	MG	BB	205	1/1	0.97	0.13	1,1,1,1	0
60	MG	AA	1675	1/1	0.97	0.16	4,4,4,4	0
60	MG	BE	301	1/1	0.97	0.09	1,1,1,1	0
60	MG	DA	3074	1/1	0.97	0.27	48,48,48,48	0
60	MG	BA	3246	1/1	0.97	0.14	1,1,1,1	0
60	MG	AA	1655	1/1	0.97	0.21	2,2,2,2	0
60	MG	AA	1606	1/1	0.97	0.17	1,1,1,1	0
60	MG	BP	201	1/1	0.97	0.22	11,11,11,11	0
60	MG	DA	3151	1/1	0.97	0.19	26,26,26,26	0
60	MG	AA	1615	1/1	0.97	0.06	18,18,18,18	0
60	MG	DA	3081	1/1	0.97	0.12	3,3,3,3	0
60	MG	BA	3095	1/1	0.97	0.19	47,47,47,47	0
60	MG	CA	1650	1/1	0.97	0.20	1,1,1,1	0
60	MG	BA	3118	1/1	0.97	0.31	46,46,46,46	0
60	MG	BA	3298	1/1	0.97	0.17	13,13,13,13	0
60	MG	BA	3181	1/1	0.97	0.20	16,16,16,16	0
60	MG	BA	3255	1/1	0.97	0.07	19,19,19,19	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	DA	3089	1/1	0.97	0.07	27,27,27,27	0
60	MG	DA	3010	1/1	0.97	0.18	1,1,1,1	0
60	MG	DA	3012	1/1	0.97	0.12	1,1,1,1	0
60	MG	AA	1627	1/1	0.97	0.16	22,22,22,22	0
60	MG	BA	3220	1/1	0.97	0.12	1,1,1,1	0
60	MG	DA	3017	1/1	0.97	0.09	1,1,1,1	0
60	MG	AA	1711	1/1	0.97	0.05	15,15,15,15	0
60	MG	DA	3019	1/1	0.97	0.04	6,6,6,6	0
60	MG	DA	3169	1/1	0.97	0.18	16,16,16,16	0
60	MG	BA	3154	1/1	0.97	0.05	16,16,16,16	0
61	ZN	D4	101	1/1	0.97	0.04	113,113,113,113	0
61	ZN	D5	102	1/1	0.97	0.04	75,75,75,75	0
60	MG	BA	3045	1/1	0.98	0.11	2,2,2,2	0
60	MG	BA	3028	1/1	0.98	0.08	1,1,1,1	0
60	MG	BA	3012	1/1	0.98	0.20	1,1,1,1	0
60	MG	CA	1661	1/1	0.98	0.08	9,9,9,9	0
60	MG	BA	3175	1/1	0.98	0.13	26,26,26,26	0
60	MG	DA	3004	1/1	0.98	0.12	7,7,7,7	0
60	MG	BA	3030	1/1	0.98	0.10	7,7,7,7	0
60	MG	DA	3006	1/1	0.98	0.26	4,4,4,4	0
60	MG	AA	1693	1/1	0.98	0.06	31,31,31,31	0
60	MG	AA	1639	1/1	0.98	0.03	29,29,29,29	0
60	MG	CA	1667	1/1	0.98	0.14	5,5,5,5	0
60	MG	DA	3011	1/1	0.98	0.06	4,4,4,4	0
60	MG	AA	1662	1/1	0.98	0.06	21,21,21,21	0
60	MG	BA	3214	1/1	0.98	0.09	54,54,54,54	0
60	MG	DA	3014	1/1	0.98	0.14	4,4,4,4	0
60	MG	DA	3015	1/1	0.98	0.09	1,1,1,1	0
60	MG	BA	3290	1/1	0.98	0.17	24,24,24,24	0
60	MG	BA	3150	1/1	0.98	0.19	9,9,9,9	0
60	MG	BA	3121	1/1	0.98	0.26	23,23,23,23	0
60	MG	BA	3182	1/1	0.98	0.10	1,1,1,1	0
60	MG	BA	3218	1/1	0.98	0.08	9,9,9,9	0
60	MG	DA	3208	1/1	0.98	0.08	12,12,12,12	0
60	MG	BA	3183	1/1	0.98	0.14	1,1,1,1	0
60	MG	DA	3022	1/1	0.98	0.07	11,11,11,11	0
60	MG	DA	3023	1/1	0.98	0.07	14,14,14,14	0
60	MG	AA	1650	1/1	0.98	0.12	15,15,15,15	0
60	MG	BA	3257	1/1	0.98	0.04	22,22,22,22	0
60	MG	CA	1678	1/1	0.98	0.26	25,25,25,25	0
60	MG	BA	3098	1/1	0.98	0.31	1,1,1,1	0
60	MG	BA	3099	1/1	0.98	0.22	8,8,8,8	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	AA	1714	1/1	0.98	0.12	6,6,6,6	0
60	MG	DA	3030	1/1	0.98	0.04	8,8,8,8	0
60	MG	BA	3055	1/1	0.98	0.11	1,1,1,1	0
60	MG	BF	301	1/1	0.98	0.04	14,14,14,14	0
60	MG	BA	3262	1/1	0.98	0.15	3,3,3,3	0
60	MG	BA	3019	1/1	0.98	0.19	1,1,1,1	0
60	MG	BP	202	1/1	0.98	0.14	1,1,1,1	0
60	MG	BA	3020	1/1	0.98	0.19	1,1,1,1	0
60	MG	BA	3038	1/1	0.98	0.19	1,1,1,1	0
60	MG	BA	3306	1/1	0.98	0.12	5,5,5,5	0
60	MG	DA	3165	1/1	0.98	0.11	14,14,14,14	0
60	MG	AA	1623	1/1	0.98	0.19	10,10,10,10	0
60	MG	DA	3230	1/1	0.98	0.04	17,17,17,17	0
60	MG	BA	3081	1/1	0.98	0.07	19,19,19,19	0
60	MG	DA	3233	1/1	0.98	0.12	1,1,1,1	0
60	MG	DA	3044	1/1	0.98	0.09	1,1,1,1	0
60	MG	AA	1641	1/1	0.98	0.10	13,13,13,13	0
60	MG	DA	3236	1/1	0.98	0.08	39,39,39,39	0
60	MG	BA	3023	1/1	0.98	0.06	1,1,1,1	0
60	MG	CA	1646	1/1	0.98	0.08	1,1,1,1	0
60	MG	AA	1611	1/1	0.98	0.07	33,33,33,33	0
60	MG	BA	3233	1/1	0.98	0.08	1,1,1,1	0
60	MG	BA	3063	1/1	0.98	0.13	1,1,1,1	0
60	MG	BA	3137	1/1	0.98	0.18	1,1,1,1	0
60	MG	BA	3275	1/1	0.98	0.10	7,7,7,7	0
60	MG	BA	3111	1/1	0.98	0.09	1,1,1,1	0
60	MG	BA	3317	1/1	0.98	0.11	22,22,22,22	0
60	MG	DA	3179	1/1	0.98	0.04	19,19,19,19	0
60	MG	BA	3318	1/1	0.98	0.04	20,20,20,20	0
60	MG	DA	3058	1/1	0.98	0.12	1,1,1,1	0
60	MG	AA	1635	1/1	0.98	0.09	23,23,23,23	0
61	ZN	AD	301	1/1	0.98	0.17	46,46,46,46	0
61	ZN	B4	101	1/1	0.98	0.04	89,89,89,89	0
60	MG	DA	3183	1/1	0.98	0.11	9,9,9,9	0
60	MG	BA	3011	1/1	0.98	0.10	1,1,1,1	0
60	MG	BA	3239	1/1	0.98	0.13	2,2,2,2	0
61	ZN	D9	101	1/1	0.98	0.04	93,93,93,93	0
60	MG	BA	3131	1/1	0.99	0.23	1,1,1,1	0
60	MG	DA	3045	1/1	0.99	0.04	11,11,11,11	0
60	MG	AA	1666	1/1	0.99	0.06	9,9,9,9	0
60	MG	AA	1667	1/1	0.99	0.05	15,15,15,15	0
60	MG	BA	3087	1/1	0.99	0.04	6,6,6,6	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	BA	3153	1/1	0.99	0.27	16,16,16,16	0
60	MG	DA	3132	1/1	0.99	0.06	6,6,6,6	0
60	MG	CA	1627	1/1	0.99	0.03	9,9,9,9	0
60	MG	CA	1689	1/1	0.99	0.03	7,7,7,7	0
60	MG	BA	3324	1/1	0.99	0.04	1,1,1,1	0
60	MG	AA	1668	1/1	0.99	0.07	24,24,24,24	0
60	MG	AA	1676	1/1	0.99	0.18	11,11,11,11	0
60	MG	BA	3156	1/1	0.99	0.07	7,7,7,7	0
60	MG	DA	3224	1/1	0.99	0.03	18,18,18,18	0
60	MG	DA	3056	1/1	0.99	0.03	2,2,2,2	0
60	MG	BA	3024	1/1	0.99	0.06	11,11,11,11	0
60	MG	BA	3199	1/1	0.99	0.11	1,1,1,1	0
60	MG	BA	3138	1/1	0.99	0.08	1,1,1,1	0
60	MG	AA	1634	1/1	0.99	0.12	1,1,1,1	0
60	MG	CA	1666	1/1	0.99	0.07	9,9,9,9	0
60	MG	BA	3277	1/1	0.99	0.05	1,1,1,1	0
60	MG	DA	3232	1/1	0.99	0.09	3,3,3,3	0
60	MG	AA	1694	1/1	0.99	0.13	5,5,5,5	0
60	MG	BA	3015	1/1	0.99	0.04	5,5,5,5	0
60	MG	DA	3106	1/1	0.99	0.03	23,23,23,23	0
60	MG	BA	3252	1/1	0.99	0.04	4,4,4,4	0
60	MG	DA	3108	1/1	0.99	0.09	18,18,18,18	0
60	MG	BA	3052	1/1	0.99	0.18	1,1,1,1	0
60	MG	BA	3254	1/1	0.99	0.08	72,72,72,72	0
60	MG	AA	1602	1/1	0.99	0.05	1,1,1,1	0
60	MG	DA	3070	1/1	0.99	0.09	14,14,14,14	0
60	MG	DA	3031	1/1	0.99	0.06	9,9,9,9	0
60	MG	BA	3206	1/1	0.99	0.19	6,6,6,6	0
60	MG	DA	3034	1/1	0.99	0.06	1,1,1,1	0
60	MG	DE	301	1/1	0.99	0.04	1,1,1,1	0
60	MG	AA	1609	1/1	0.99	0.13	1,1,1,1	0
60	MG	BA	3208	1/1	0.99	0.17	1,1,1,1	0
60	MG	BA	3185	1/1	0.99	0.05	3,3,3,3	0
60	MG	DA	3077	1/1	0.99	0.05	13,13,13,13	0
60	MG	AX	105	1/1	0.99	0.03	12,12,12,12	0
60	MG	AA	1624	1/1	0.99	0.19	1,1,1,1	0
60	MG	DA	3206	1/1	0.99	0.05	12,12,12,12	0
60	MG	BA	3070	1/1	0.99	0.31	1,1,1,1	0
61	ZN	CD	301	1/1	0.99	0.19	49,49,49,49	0
60	MG	CA	1620	1/1	0.99	0.10	32,32,32,32	0
60	MG	BA	3148	1/1	0.99	0.05	1,1,1,1	0
60	MG	DA	3007	1/1	0.99	0.05	1,1,1,1	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	DA	3061	1/1	1.00	0.02	21,21,21,21	0
60	MG	BA	3090	1/1	1.00	0.04	13,13,13,13	0
60	MG	DA	3032	1/1	1.00	0.02	1,1,1,1	0
60	MG	DA	3085	1/1	1.00	0.21	1,1,1,1	0
61	ZN	B9	101	1/1	1.00	0.02	44,44,44,44	0
60	MG	BR	201	1/1	1.00	0.03	1,1,1,1	0
60	MG	BA	3273	1/1	1.00	0.03	1,1,1,1	0
60	MG	AX	107	1/1	1.00	0.05	8,8,8,8	0
60	MG	CK	201	1/1	1.00	0.03	19,19,19,19	0

5.5 Other polymers [i](#)

There are no such residues in this entry.