



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 17, 2026 – 01:55 AM UTC

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

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

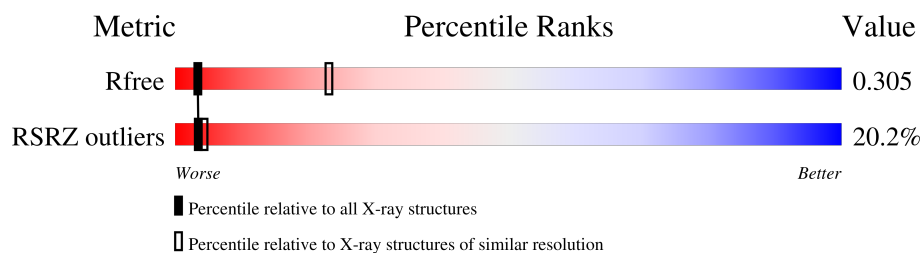
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.46 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1597 (3.52-3.40)
RSRZ outliers	164620	1596 (3.52-3.40)

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

2 Entry composition

There are 54 unique types of molecules in this entry. The entry contains 284107 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 54 is water.

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

Continued on next page...

Continued from previous page...

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

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

3 Data and refinement statistics

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

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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

4.2 Too-close contacts [i](#)

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

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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

4.3.2 Protein sidechains [i](#)

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

4.3.3 RNA [i](#)

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

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

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
21	AU	2
21	CU	1

All chain breaks are listed below:

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

5 Fit of model and data ⓘ

5.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1530/1542 (99%)	0.72	98 (6%) 27 22	16, 66, 135, 180	0
1	CA	1530/1542 (99%)	0.40	63 (4%) 42 31	11, 49, 119, 180	0
2	AC	206/232 (88%)	0.66	18 (8%) 17 15	8, 56, 116, 163	0
2	CC	206/232 (88%)	0.79	22 (10%) 12 12	13, 68, 122, 154	0
3	AD	205/205 (100%)	1.15	45 (21%) 3 4	16, 65, 125, 180	0
3	CD	205/205 (100%)	0.69	20 (9%) 14 13	5, 49, 103, 156	0
4	AE	150/166 (90%)	0.78	11 (7%) 22 19	5, 56, 104, 151	0
4	CE	150/166 (90%)	0.52	13 (8%) 17 15	5, 49, 101, 167	0
5	AF	100/135 (74%)	0.73	8 (8%) 20 17	19, 64, 113, 150	0
5	CF	100/135 (74%)	1.04	18 (18%) 4 5	10, 65, 113, 147	0
6	AG	150/178 (84%)	1.03	25 (16%) 5 6	23, 86, 133, 180	0
6	CG	152/178 (85%)	0.86	17 (11%) 11 11	22, 83, 132, 166	0
7	AH	129/129 (100%)	0.87	16 (12%) 9 9	8, 63, 113, 155	0
7	CH	129/129 (100%)	0.82	14 (10%) 12 12	5, 49, 104, 154	0
8	AI	127/129 (98%)	1.16	23 (18%) 4 5	5, 83, 126, 169	0
8	CI	127/129 (98%)	1.41	31 (24%) 2 3	22, 81, 135, 161	0
9	AJ	98/103 (95%)	1.23	18 (18%) 4 5	14, 76, 141, 160	0
9	CJ	98/103 (95%)	1.23	21 (21%) 3 4	27, 78, 122, 143	0
10	AK	117/128 (91%)	0.94	15 (12%) 9 9	6, 56, 99, 164	0
10	CK	117/128 (91%)	0.63	9 (7%) 21 18	5, 44, 95, 117	0
11	AL	123/123 (100%)	1.23	30 (24%) 2 3	18, 59, 115, 162	0
11	CL	123/123 (100%)	0.68	18 (14%) 7 8	5, 34, 109, 141	0
12	AM	114/117 (97%)	1.28	25 (21%) 3 4	37, 96, 137, 155	0
12	CM	113/117 (96%)	1.20	21 (18%) 4 5	19, 92, 143, 180	0

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

The worst 5 of 4131 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
42	BU	29	SER	15.0
45	BY	3	THR	14.8
26	BD	134	HIS	13.6
42	BU	89	GLY	13.0
33	BL	82	LEU	12.9

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

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

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
53	MG	AA	1636	1/1	0.55	0.37	127,127,127,127	0
53	MG	DB	3059	1/1	0.61	0.14	127,127,127,127	0
53	MG	AA	1649	1/1	0.67	0.16	114,114,114,114	0
53	MG	CA	1623	1/1	0.68	0.14	151,151,151,151	0
53	MG	AA	1612	1/1	0.71	0.16	104,104,104,104	0
53	MG	AA	1629	1/1	0.72	0.18	138,138,138,138	0
53	MG	AA	1622	1/1	0.78	0.14	116,116,116,116	0
53	MG	BB	3067	1/1	0.78	0.15	78,78,78,78	0
53	MG	AA	1644	1/1	0.81	0.12	96,96,96,96	0
53	MG	AA	1619	1/1	0.82	0.13	100,100,100,100	0
53	MG	DB	3082	1/1	0.83	0.15	73,73,73,73	0
53	MG	AA	1638	1/1	0.84	0.16	98,98,98,98	0
53	MG	AA	1658	1/1	0.84	0.16	167,167,167,167	0
53	MG	AA	1623	1/1	0.85	0.23	32,32,32,32	1
53	MG	AP	101	1/1	0.85	0.19	53,53,53,53	1
53	MG	CA	1616	1/1	0.86	0.18	68,68,68,68	0
53	MG	BB	3042	1/1	0.88	0.07	95,95,95,95	0
53	MG	CA	1615	1/1	0.88	0.11	101,101,101,101	0
53	MG	BB	3081	1/1	0.89	0.10	46,46,46,46	0
53	MG	BB	3082	1/1	0.89	0.12	19,19,19,19	0
53	MG	DB	3034	1/1	0.89	0.14	66,66,66,66	0
53	MG	BB	3090	1/1	0.89	0.08	74,74,74,74	0
53	MG	AA	1608	1/1	0.89	0.12	121,121,121,121	0
53	MG	BB	3110	1/1	0.90	0.15	60,60,60,60	0
53	MG	BB	3063	1/1	0.90	0.11	27,27,27,27	0
53	MG	CA	1628	1/1	0.90	0.13	55,55,55,55	1
53	MG	AA	1655	1/1	0.91	0.14	75,75,75,75	0
53	MG	CA	1621	1/1	0.91	0.15	113,113,113,113	0
53	MG	DB	3013	1/1	0.91	0.12	34,34,34,34	0
53	MG	BB	3060	1/1	0.92	0.08	69,69,69,69	0
53	MG	BB	3021	1/1	0.92	0.12	55,55,55,55	0
53	MG	AA	1614	1/1	0.92	0.09	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	DB	3065	1/1	0.92	0.26	47,47,47,47	1
53	MG	CA	1632	1/1	0.92	0.09	61,61,61,61	0
53	MG	CA	1639	1/1	0.93	0.07	117,117,117,117	0
53	MG	AA	1659	1/1	0.93	0.07	105,105,105,105	0
53	MG	DB	3024	1/1	0.93	0.11	36,36,36,36	0
53	MG	BB	3088	1/1	0.93	0.13	34,34,34,34	0
53	MG	BB	3026	1/1	0.93	0.08	5,5,5,5	0
53	MG	DB	3060	1/1	0.93	0.08	77,77,77,77	0
53	MG	BB	3033	1/1	0.93	0.10	93,93,93,93	0
53	MG	AA	1641	1/1	0.93	0.09	49,49,49,49	0
53	MG	DB	3091	1/1	0.93	0.08	96,96,96,96	0
53	MG	DB	3104	1/1	0.93	0.07	50,50,50,50	0
53	MG	CA	1634	1/1	0.94	0.10	61,61,61,61	0
53	MG	AA	1657	1/1	0.94	0.09	81,81,81,81	0
53	MG	CA	1648	1/1	0.94	0.14	56,56,56,56	0
53	MG	CA	1660	1/1	0.94	0.09	65,65,65,65	0
53	MG	BB	3094	1/1	0.94	0.06	35,35,35,35	0
53	MG	AA	1654	1/1	0.94	0.10	59,59,59,59	0
53	MG	DB	3103	1/1	0.94	0.09	50,50,50,50	0
53	MG	DB	3030	1/1	0.94	0.09	23,23,23,23	0
53	MG	AA	1637	1/1	0.95	0.08	81,81,81,81	0
53	MG	BB	3074	1/1	0.95	0.09	13,13,13,13	0
53	MG	BB	3093	1/1	0.95	0.20	5,5,5,5	1
53	MG	CA	1627	1/1	0.95	0.13	29,29,29,29	1
53	MG	BB	3079	1/1	0.95	0.11	38,38,38,38	0
53	MG	BB	3096	1/1	0.95	0.07	43,43,43,43	0
53	MG	AA	1639	1/1	0.95	0.06	47,47,47,47	0
53	MG	CA	1637	1/1	0.95	0.10	68,68,68,68	0
53	MG	CA	1608	1/1	0.95	0.12	110,110,110,110	0
53	MG	BB	3034	1/1	0.95	0.08	25,25,25,25	0
53	MG	CA	1649	1/1	0.95	0.14	88,88,88,88	0
53	MG	CA	1650	1/1	0.95	0.09	82,82,82,82	0
53	MG	BB	3046	1/1	0.96	0.07	51,51,51,51	0
53	MG	BB	3047	1/1	0.96	0.06	114,114,114,114	0
53	MG	CA	1645	1/1	0.96	0.12	82,82,82,82	0
53	MG	AA	1617	1/1	0.96	0.07	78,78,78,78	0
53	MG	BB	3100	1/1	0.96	0.17	11,11,11,11	1
53	MG	BB	3010	1/1	0.96	0.09	39,39,39,39	0
53	MG	BB	3017	1/1	0.96	0.08	72,72,72,72	0
53	MG	CA	1611	1/1	0.96	0.07	71,71,71,71	0
53	MG	CA	1613	1/1	0.96	0.08	78,78,78,78	0
53	MG	AA	1624	1/1	0.96	0.15	79,79,79,79	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	BB	3077	1/1	0.96	0.09	44,44,44,44	0
53	MG	DB	3058	1/1	0.96	0.10	30,30,30,30	1
53	MG	BB	3078	1/1	0.96	0.18	25,25,25,25	0
53	MG	AA	1605	1/1	0.96	0.07	48,48,48,48	0
53	MG	CA	1624	1/1	0.96	0.09	48,48,48,48	0
53	MG	BB	3028	1/1	0.96	0.10	40,40,40,40	0
53	MG	AA	1635	1/1	0.96	0.08	85,85,85,85	0
53	MG	AA	1602	1/1	0.96	0.05	62,62,62,62	0
53	MG	AA	1648	1/1	0.96	0.06	94,94,94,94	0
53	MG	AA	1632	1/1	0.97	0.05	53,53,53,53	0
53	MG	BB	3051	1/1	0.97	0.06	71,71,71,71	0
53	MG	CA	1636	1/1	0.97	0.09	51,51,51,51	0
53	MG	AA	1633	1/1	0.97	0.05	75,75,75,75	0
53	MG	AA	1634	1/1	0.97	0.09	85,85,85,85	0
53	MG	CA	1641	1/1	0.97	0.14	92,92,92,92	0
53	MG	CA	1643	1/1	0.97	0.06	41,41,41,41	0
53	MG	BB	3098	1/1	0.97	0.08	45,45,45,45	0
53	MG	BB	3065	1/1	0.97	0.08	47,47,47,47	0
53	MG	BB	3105	1/1	0.97	0.16	64,64,64,64	0
53	MG	AA	1604	1/1	0.97	0.08	45,45,45,45	0
53	MG	CA	1657	1/1	0.97	0.06	37,37,37,37	0
53	MG	CA	1603	1/1	0.97	0.11	69,69,69,69	0
53	MG	CA	1662	1/1	0.97	0.09	26,26,26,26	0
53	MG	CA	1606	1/1	0.97	0.06	74,74,74,74	0
53	MG	DB	3015	1/1	0.97	0.06	49,49,49,49	0
53	MG	BB	3030	1/1	0.97	0.05	53,53,53,53	0
53	MG	BB	3075	1/1	0.97	0.11	31,31,31,31	0
53	MG	AA	1611	1/1	0.97	0.07	40,40,40,40	0
53	MG	DB	3050	1/1	0.97	0.08	74,74,74,74	0
53	MG	DB	3051	1/1	0.97	0.08	53,53,53,53	0
53	MG	DB	3052	1/1	0.97	0.17	60,60,60,60	0
53	MG	DB	3053	1/1	0.97	0.15	27,27,27,27	0
53	MG	AA	1631	1/1	0.97	0.10	61,61,61,61	0
53	MG	BB	3041	1/1	0.97	0.05	30,30,30,30	0
53	MG	BB	3007	1/1	0.97	0.08	28,28,28,28	0
53	MG	DB	3061	1/1	0.97	0.04	78,78,78,78	0
53	MG	BB	3043	1/1	0.97	0.09	75,75,75,75	0
53	MG	DB	3077	1/1	0.97	0.08	57,57,57,57	0
53	MG	BB	3087	1/1	0.97	0.10	45,45,45,45	0
53	MG	DB	3083	1/1	0.97	0.14	27,27,27,27	0
53	MG	DB	3088	1/1	0.97	0.09	35,35,35,35	0
53	MG	DB	3089	1/1	0.97	0.05	65,65,65,65	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	CA	1626	1/1	0.97	0.06	73,73,73,73	0
53	MG	DB	3095	1/1	0.97	0.11	55,55,55,55	0
53	MG	AA	1653	1/1	0.97	0.07	65,65,65,65	0
53	MG	BB	3089	1/1	0.97	0.07	45,45,45,45	0
53	MG	DB	3110	1/1	0.97	0.11	54,54,54,54	0
53	MG	AA	1606	1/1	0.98	0.04	59,59,59,59	0
53	MG	AA	1650	1/1	0.98	0.07	72,72,72,72	0
53	MG	CA	1635	1/1	0.98	0.05	20,20,20,20	0
53	MG	AA	1651	1/1	0.98	0.06	84,84,84,84	0
53	MG	AA	1625	1/1	0.98	0.06	5,5,5,5	1
53	MG	BB	3039	1/1	0.98	0.11	45,45,45,45	0
53	MG	AA	1626	1/1	0.98	0.07	35,35,35,35	0
53	MG	CA	1642	1/1	0.98	0.06	45,45,45,45	0
53	MG	BB	3091	1/1	0.98	0.08	19,19,19,19	0
53	MG	AA	1627	1/1	0.98	0.10	72,72,72,72	0
53	MG	AA	1656	1/1	0.98	0.16	66,66,66,66	0
53	MG	AA	1628	1/1	0.98	0.06	26,26,26,26	0
53	MG	BB	3097	1/1	0.98	0.09	74,74,74,74	0
53	MG	CA	1652	1/1	0.98	0.08	44,44,44,44	0
53	MG	AA	1607	1/1	0.98	0.06	27,27,27,27	0
53	MG	CA	1659	1/1	0.98	0.17	48,48,48,48	0
53	MG	BB	3099	1/1	0.98	0.05	30,30,30,30	0
53	MG	CA	1661	1/1	0.98	0.04	62,62,62,62	0
53	MG	BB	3049	1/1	0.98	0.08	11,11,11,11	0
53	MG	DB	3001	1/1	0.98	0.08	7,7,7,7	0
53	MG	DB	3002	1/1	0.98	0.06	37,37,37,37	0
53	MG	BB	3101	1/1	0.98	0.07	12,12,12,12	0
53	MG	AA	1620	1/1	0.98	0.09	62,62,62,62	0
53	MG	DB	3016	1/1	0.98	0.05	23,23,23,23	0
53	MG	DB	3020	1/1	0.98	0.07	20,20,20,20	0
53	MG	BB	3107	1/1	0.98	0.07	27,27,27,27	0
53	MG	DB	3027	1/1	0.98	0.08	10,10,10,10	0
53	MG	DB	3029	1/1	0.98	0.17	41,41,41,41	0
53	MG	BB	3109	1/1	0.98	0.13	15,15,15,15	0
53	MG	BB	3052	1/1	0.98	0.10	19,19,19,19	0
53	MG	DB	3041	1/1	0.98	0.06	18,18,18,18	0
53	MG	DB	3045	1/1	0.98	0.04	61,61,61,61	0
53	MG	DB	3047	1/1	0.98	0.07	17,17,17,17	0
53	MG	BB	3054	1/1	0.98	0.06	72,72,72,72	0
53	MG	AA	1642	1/1	0.98	0.05	70,70,70,70	0
53	MG	AA	1643	1/1	0.98	0.05	73,73,73,73	0
53	MG	CA	1609	1/1	0.98	0.12	45,45,45,45	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	DB	3057	1/1	0.98	0.06	28,28,28,28	0
53	MG	BB	3009	1/1	0.98	0.07	35,35,35,35	0
53	MG	AA	1603	1/1	0.98	0.05	43,43,43,43	0
53	MG	CA	1614	1/1	0.98	0.08	47,47,47,47	0
53	MG	BB	3071	1/1	0.98	0.05	24,24,24,24	0
53	MG	DB	3062	1/1	0.98	0.08	43,43,43,43	0
53	MG	BB	3072	1/1	0.98	0.06	24,24,24,24	0
53	MG	DB	3067	1/1	0.98	0.04	17,17,17,17	0
53	MG	DB	3071	1/1	0.98	0.07	39,39,39,39	0
53	MG	DB	3076	1/1	0.98	0.05	17,17,17,17	0
53	MG	BB	3013	1/1	0.98	0.07	31,31,31,31	0
53	MG	CA	1622	1/1	0.98	0.07	67,67,67,67	0
53	MG	AA	1645	1/1	0.98	0.10	27,27,27,27	0
53	MG	AA	1646	1/1	0.98	0.13	60,60,60,60	0
53	MG	CA	1625	1/1	0.98	0.08	26,26,26,26	0
53	MG	AA	1615	1/1	0.98	0.15	43,43,43,43	0
53	MG	DB	3094	1/1	0.98	0.20	5,5,5,5	1
53	MG	BB	3027	1/1	0.98	0.11	23,23,23,23	0
53	MG	DB	3102	1/1	0.98	0.05	26,26,26,26	0
53	MG	BB	3080	1/1	0.98	0.07	31,31,31,31	0
53	MG	CA	1630	1/1	0.98	0.10	5,5,5,5	1
53	MG	DB	3107	1/1	0.98	0.06	19,19,19,19	0
53	MG	CA	1631	1/1	0.98	0.07	36,36,36,36	0
53	MG	DN	201	1/1	0.98	0.12	49,49,49,49	0
53	MG	AA	1601	1/1	0.99	0.05	26,26,26,26	0
53	MG	CA	1646	1/1	0.99	0.04	42,42,42,42	0
53	MG	CA	1647	1/1	0.99	0.05	32,32,32,32	0
53	MG	BB	3095	1/1	0.99	0.03	34,34,34,34	0
53	MG	BB	3018	1/1	0.99	0.04	27,27,27,27	0
53	MG	BB	3048	1/1	0.99	0.04	20,20,20,20	0
53	MG	CA	1651	1/1	0.99	0.02	14,14,14,14	0
53	MG	BB	3019	1/1	0.99	0.09	27,27,27,27	0
53	MG	CA	1653	1/1	0.99	0.17	45,45,45,45	0
53	MG	CA	1654	1/1	0.99	0.04	40,40,40,40	0
53	MG	CA	1655	1/1	0.99	0.10	48,48,48,48	0
53	MG	CA	1656	1/1	0.99	0.10	48,48,48,48	0
53	MG	BB	3050	1/1	0.99	0.05	35,35,35,35	0
53	MG	CA	1658	1/1	0.99	0.10	38,38,38,38	0
53	MG	AA	1640	1/1	0.99	0.09	44,44,44,44	0
53	MG	BB	3022	1/1	0.99	0.03	38,38,38,38	0
53	MG	BB	3102	1/1	0.99	0.04	19,19,19,19	0
53	MG	BB	3104	1/1	0.99	0.04	18,18,18,18	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	BB	3024	1/1	0.99	0.03	22,22,22,22	0
53	MG	BB	3106	1/1	0.99	0.06	46,46,46,46	0
53	MG	DB	3003	1/1	0.99	0.04	14,14,14,14	0
53	MG	DB	3004	1/1	0.99	0.07	19,19,19,19	0
53	MG	DB	3007	1/1	0.99	0.04	12,12,12,12	0
53	MG	DB	3008	1/1	0.99	0.07	24,24,24,24	0
53	MG	BB	3055	1/1	0.99	0.06	27,27,27,27	0
53	MG	DB	3014	1/1	0.99	0.05	5,5,5,5	0
53	MG	BB	3108	1/1	0.99	0.06	19,19,19,19	0
53	MG	BB	3057	1/1	0.99	0.14	27,27,27,27	0
53	MG	DB	3018	1/1	0.99	0.04	29,29,29,29	0
53	MG	BB	3058	1/1	0.99	0.04	28,28,28,28	0
53	MG	DB	3022	1/1	0.99	0.05	15,15,15,15	0
53	MG	CA	1602	1/1	0.99	0.11	32,32,32,32	0
53	MG	DB	3025	1/1	0.99	0.06	21,21,21,21	0
53	MG	DB	3026	1/1	0.99	0.12	18,18,18,18	0
53	MG	BB	3059	1/1	0.99	0.03	10,10,10,10	0
53	MG	DB	3028	1/1	0.99	0.05	28,28,28,28	0
53	MG	BB	3025	1/1	0.99	0.07	53,53,53,53	0
53	MG	CA	1607	1/1	0.99	0.05	18,18,18,18	0
53	MG	DB	3031	1/1	0.99	0.05	18,18,18,18	0
53	MG	DB	3032	1/1	0.99	0.04	46,46,46,46	0
53	MG	BB	3061	1/1	0.99	0.06	42,42,42,42	0
53	MG	DB	3035	1/1	0.99	0.11	30,30,30,30	0
53	MG	DB	3036	1/1	0.99	0.03	16,16,16,16	0
53	MG	DB	3037	1/1	0.99	0.04	13,13,13,13	0
53	MG	DB	3040	1/1	0.99	0.06	5,5,5,5	0
53	MG	AA	1610	1/1	0.99	0.05	34,34,34,34	0
53	MG	DB	3042	1/1	0.99	0.04	27,27,27,27	0
53	MG	DB	3043	1/1	0.99	0.07	9,9,9,9	0
53	MG	BB	3064	1/1	0.99	0.07	39,39,39,39	0
53	MG	DB	3046	1/1	0.99	0.04	33,33,33,33	0
53	MG	CA	1612	1/1	0.99	0.07	29,29,29,29	0
53	MG	AA	1621	1/1	0.99	0.05	23,23,23,23	0
53	MG	BB	3066	1/1	0.99	0.05	59,59,59,59	0
53	MG	BB	3005	1/1	0.99	0.07	5,5,5,5	0
53	MG	BB	3068	1/1	0.99	0.04	24,24,24,24	0
53	MG	DB	3054	1/1	0.99	0.06	15,15,15,15	0
53	MG	DB	3055	1/1	0.99	0.03	19,19,19,19	0
53	MG	CA	1620	1/1	0.99	0.03	35,35,35,35	0
53	MG	BB	3029	1/1	0.99	0.06	13,13,13,13	0
53	MG	AA	1616	1/1	0.99	0.04	46,46,46,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	BB	3073	1/1	0.99	0.03	28,28,28,28	0
53	MG	BB	3031	1/1	0.99	0.17	45,45,45,45	0
53	MG	BB	3032	1/1	0.99	0.07	9,9,9,9	0
53	MG	BB	3008	1/1	0.99	0.04	58,58,58,58	0
53	MG	AA	1613	1/1	0.99	0.03	42,42,42,42	0
53	MG	DB	3068	1/1	0.99	0.06	14,14,14,14	0
53	MG	DB	3069	1/1	0.99	0.04	44,44,44,44	0
53	MG	DB	3070	1/1	0.99	0.04	46,46,46,46	0
53	MG	BB	3035	1/1	0.99	0.04	12,12,12,12	0
53	MG	DB	3072	1/1	0.99	0.04	30,30,30,30	0
53	MG	DB	3073	1/1	0.99	0.03	16,16,16,16	0
53	MG	CA	1629	1/1	0.99	0.05	45,45,45,45	0
53	MG	BB	3036	1/1	0.99	0.07	37,37,37,37	0
53	MG	DB	3078	1/1	0.99	0.03	18,18,18,18	0
53	MG	BB	3037	1/1	0.99	0.03	24,24,24,24	0
53	MG	BB	3038	1/1	0.99	0.03	58,58,58,58	0
53	MG	DB	3086	1/1	0.99	0.09	69,69,69,69	0
53	MG	DB	3087	1/1	0.99	0.03	6,6,6,6	0
53	MG	CA	1633	1/1	0.99	0.05	47,47,47,47	0
53	MG	BB	3083	1/1	0.99	0.04	20,20,20,20	0
53	MG	BB	3086	1/1	0.99	0.08	37,37,37,37	0
53	MG	AA	1630	1/1	0.99	0.04	30,30,30,30	0
53	MG	BB	3040	1/1	0.99	0.05	21,21,21,21	0
53	MG	DB	3096	1/1	0.99	0.04	20,20,20,20	0
53	MG	DB	3098	1/1	0.99	0.05	18,18,18,18	0
53	MG	DB	3099	1/1	0.99	0.04	9,9,9,9	0
53	MG	CA	1638	1/1	0.99	0.05	37,37,37,37	0
53	MG	BB	3012	1/1	0.99	0.05	41,41,41,41	0
53	MG	AA	1618	1/1	0.99	0.04	46,46,46,46	0
53	MG	DB	3105	1/1	0.99	0.06	23,23,23,23	0
53	MG	DB	3106	1/1	0.99	0.06	21,21,21,21	0
53	MG	BB	3016	1/1	0.99	0.10	15,15,15,15	0
53	MG	DB	3109	1/1	0.99	0.04	24,24,24,24	0
53	MG	BB	3045	1/1	0.99	0.07	31,31,31,31	0
53	MG	CA	1644	1/1	0.99	0.04	29,29,29,29	0
53	MG	BB	3085	1/1	1.00	0.02	22,22,22,22	0
53	MG	BB	3020	1/1	1.00	0.02	23,23,23,23	0
53	MG	DB	3048	1/1	1.00	0.07	20,20,20,20	0
53	MG	DB	3049	1/1	1.00	0.02	5,5,5,5	0
53	MG	CA	1601	1/1	1.00	0.02	5,5,5,5	0
53	MG	BB	3001	1/1	1.00	0.03	10,10,10,10	0
53	MG	BB	3002	1/1	1.00	0.03	10,10,10,10	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	DB	3005	1/1	1.00	0.02	9,9,9,9	0
53	MG	DB	3006	1/1	1.00	0.02	5,5,5,5	0
53	MG	CA	1604	1/1	1.00	0.04	18,18,18,18	0
53	MG	DB	3056	1/1	1.00	0.01	11,11,11,11	0
53	MG	CA	1605	1/1	1.00	0.03	18,18,18,18	0
53	MG	DB	3009	1/1	1.00	0.03	7,7,7,7	0
53	MG	DB	3010	1/1	1.00	0.02	12,12,12,12	0
53	MG	DB	3011	1/1	1.00	0.02	8,8,8,8	0
53	MG	DB	3012	1/1	1.00	0.05	6,6,6,6	0
53	MG	BB	3023	1/1	1.00	0.02	22,22,22,22	0
53	MG	DB	3063	1/1	1.00	0.09	13,13,13,13	0
53	MG	DB	3064	1/1	1.00	0.06	28,28,28,28	0
53	MG	BB	3011	1/1	1.00	0.06	7,7,7,7	0
53	MG	DB	3066	1/1	1.00	0.05	5,5,5,5	0
53	MG	BB	3069	1/1	1.00	0.03	9,9,9,9	0
53	MG	CA	1640	1/1	1.00	0.02	11,11,11,11	0
53	MG	DB	3017	1/1	1.00	0.03	5,5,5,5	0
53	MG	BB	3092	1/1	1.00	0.02	11,11,11,11	0
53	MG	DB	3019	1/1	1.00	0.06	5,5,5,5	0
53	MG	CA	1610	1/1	1.00	0.02	34,34,34,34	0
53	MG	DB	3021	1/1	1.00	0.03	16,16,16,16	0
53	MG	DB	3074	1/1	1.00	0.03	25,25,25,25	0
53	MG	DB	3075	1/1	1.00	0.05	5,5,5,5	0
53	MG	BB	3070	1/1	1.00	0.02	32,32,32,32	0
53	MG	DB	3023	1/1	1.00	0.03	34,34,34,34	0
53	MG	BB	3003	1/1	1.00	0.02	13,13,13,13	0
53	MG	DB	3079	1/1	1.00	0.02	5,5,5,5	0
53	MG	DB	3080	1/1	1.00	0.03	12,12,12,12	0
53	MG	DB	3081	1/1	1.00	0.04	25,25,25,25	0
53	MG	BB	3053	1/1	1.00	0.02	6,6,6,6	0
53	MG	BB	3004	1/1	1.00	0.04	21,21,21,21	0
53	MG	DB	3084	1/1	1.00	0.02	8,8,8,8	0
53	MG	DB	3085	1/1	1.00	0.03	17,17,17,17	0
53	MG	BB	3014	1/1	1.00	0.03	29,29,29,29	0
53	MG	BB	3056	1/1	1.00	0.12	19,19,19,19	0
53	MG	CA	1617	1/1	1.00	0.02	9,9,9,9	0
53	MG	CA	1618	1/1	1.00	0.02	5,5,5,5	0
53	MG	DB	3090	1/1	1.00	0.05	28,28,28,28	0
53	MG	CA	1619	1/1	1.00	0.09	26,26,26,26	0
53	MG	DB	3092	1/1	1.00	0.02	23,23,23,23	0
53	MG	DB	3093	1/1	1.00	0.06	10,10,10,10	0
53	MG	BB	3076	1/1	1.00	0.03	24,24,24,24	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	DB	3033	1/1	1.00	0.04	11,11,11,11	0
53	MG	BB	3015	1/1	1.00	0.02	24,24,24,24	0
53	MG	DB	3097	1/1	1.00	0.06	15,15,15,15	0
53	MG	AA	1652	1/1	1.00	0.04	25,25,25,25	0
53	MG	BB	3006	1/1	1.00	0.02	10,10,10,10	0
53	MG	DB	3100	1/1	1.00	0.04	11,11,11,11	0
53	MG	DB	3101	1/1	1.00	0.04	27,27,27,27	0
53	MG	BB	3103	1/1	1.00	0.03	7,7,7,7	0
53	MG	DB	3038	1/1	1.00	0.03	16,16,16,16	0
53	MG	DB	3039	1/1	1.00	0.03	19,19,19,19	0
53	MG	BB	3044	1/1	1.00	0.04	32,32,32,32	0
53	MG	AA	1609	1/1	1.00	0.05	8,8,8,8	0
53	MG	BB	3062	1/1	1.00	0.03	22,22,22,22	0
53	MG	DB	3108	1/1	1.00	0.03	5,5,5,5	0
53	MG	AA	1647	1/1	1.00	0.02	23,23,23,23	0
53	MG	DB	3044	1/1	1.00	0.04	7,7,7,7	0
53	MG	BB	3084	1/1	1.00	0.05	5,5,5,5	0

5.5 Other polymers [i](#)

There are no such residues in this entry.