



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 18, 2026 – 12:22 PM UTC

PDB ID : 8FOM / pdb_00008fom
Title : Crystal structure of tRNA^{Lys}(SUU) bound to UAA codon in the ribosomal P site
Authors : Nguyen, H.A.; Hoffer, E.D.; Maehigashi, T.; Fagan, C.E.; Dunham, C.M.
Deposited on : 2023-01-02
Resolution : 3.58 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**
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

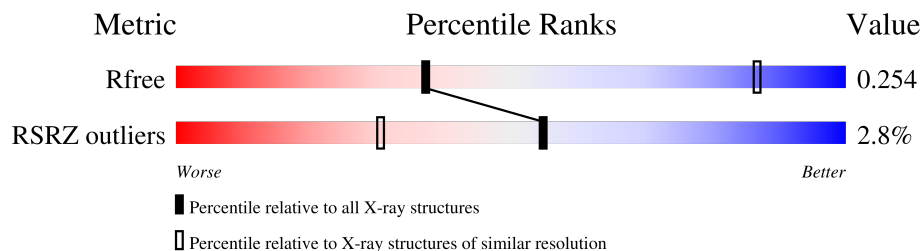
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.58 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	1521 (3.66-3.50)
RSRZ outliers	180081	1520 (3.66-3.50)

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
57	MG	YA	3300	-	-	-	X
57	MG	YA	3358	-	-	-	X

2 Entry composition [i](#)

There are 59 unique types of molecules in this entry. The entry contains 292176 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	QA	1500	Total 32247	C 14353	N 5981	O 10414	P 1499	0	0	0
1	XA	1511	Total 32471	C 14454	N 6014	O 10493	P 1510	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	QB	237	Total 1924	C 1228	N 344	O 347	S 5	0	0	0
2	XB	237	Total 1924	C 1228	N 344	O 347	S 5	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	QC	205	Total 1605	C 1011	N 313	O 280	S 1	0	0	0
3	XC	205	Total 1605	C 1011	N 313	O 280	S 1	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	QE	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			
5	XE	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	QF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
6	XF	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	QG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
7	XG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	QH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
8	XH	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	QI	127	Total	C	N	O	0	0	0
			1010	639	197	174			
9	XI	127	Total	C	N	O	0	0	0
			1010	639	197	174			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	QJ	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	XJ	99	801	504	157	139	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	QK	119	885	549	168	165	3	0	0	0
11	XK	119	885	549	168	165	3	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	QL	125	975	614	196	164	1	0	0	0
12	XL	125	975	614	196	164	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	QM	121	964	597	199	166	2	0	0	0
13	XM	121	964	597	199	166	2	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	QO	88	734	459	147	126	2	0	0	0
15	XO	88	734	459	147	126	2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	QP	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			
16	XP	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	QQ	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			
17	XQ	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	QR	70	Total	C	N	O	0	0	0
			574	367	112	95			
18	XR	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	QS	84	Total	C	N	O	S	0	0	0
			674	430	126	116	2			
19	XS	84	Total	C	N	O	S	0	0	0
			674	430	126	116	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	QT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			
20	XT	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	QU	25	Total	C	N	O	0	0	0
			217	134	52	31			
21	XU	25	Total	C	N	O	0	0	0
			217	134	52	31			

- Molecule 22 is a RNA chain called P-site tRNA^{Lys}(SUU).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	QV	74	Total	C	N	O	P	0	0	0
			1594	717	279	525	73			
22	XV	74	Total	C	N	O	P	0	0	0
			1594	717	279	525	73			

- Molecule 23 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QX	3	Total	C	N	O	P	0	0	0
			65	29	12	21	3			
23	XX	23	Total	C	N	O	P	0	0	0
			502	224	98	157	23			

- Molecule 24 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	R0	82	Total	C	N	O	S	0	0	0
			648	401	138	108	1			
24	Y0	82	Total	C	N	O	S	0	0	0
			648	401	138	108	1			

- Molecule 25 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	R1	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			
25	Y1	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			

- Molecule 26 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	R2	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
26	Y2	71	598	370	121	106	1	0	0	0

- Molecule 27 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
			Total	C	N	O				
27	R3	59	469	298	90	81		0	0	0
27	Y3	59	469	298	90	81		0	0	0

- Molecule 28 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
28	R4	71	581	364	108	104	5	0	0	0
28	Y4	71	581	364	108	104	5	0	0	0

- Molecule 29 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
29	R5	59	459	288	90	76	5	0	0	0
29	Y5	59	459	288	90	76	5	0	0	0

- Molecule 30 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
30	R6	49	424	264	87	69	4	0	0	0
30	Y6	49	424	264	87	69	4	0	0	0

- Molecule 31 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
31	R7	49	430	263	108	57	2	0	0	0
31	Y7	49	430	263	108	57	2	0	0	0

- Molecule 32 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
32	R8	64	Total 517	C 331	N 102	O 82	S 2	0	0	0
32	Y8	64	Total 517	C 331	N 102	O 82	S 2	0	0	0

- Molecule 33 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
33	R9	37	Total 307	C 188	N 68	O 47	S 4	0	0	0
33	Y9	37	Total 307	C 188	N 68	O 47	S 4	0	0	0

- Molecule 34 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
34	RA	2882	Total 62071	C 27627	N 11611	O 19952	P 2881	0	0	0
34	YA	2883	Total 62091	C 27636	N 11613	O 19960	P 2882	0	0	0

- Molecule 35 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
35	RB	120	Total 2573	C 1146	N 476	O 832	P 119	0	0	0
35	YB	120	Total 2573	C 1146	N 476	O 832	P 119	0	0	0

- Molecule 36 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
36	RD	272	Total 2115	C 1335	N 420	O 357	S 3	0	0	0
36	YD	272	Total 2115	C 1335	N 420	O 357	S 3	0	0	0

- Molecule 37 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	RE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			
37	YE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			

- Molecule 38 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	RF	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			
38	YF	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			

- Molecule 39 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	RG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			
39	YG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			

- Molecule 40 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	RH	170	Total	C	N	O	S	0	0	0
			1307	829	245	232	1			
40	YH	170	Total	C	N	O	S	0	0	0
			1307	829	245	232	1			

- Molecule 41 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	RI	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			
41	YI	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

- Molecule 42 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	RN	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
42	YN	138	1104	712	206	182	4	0	0	0

- Molecule 43 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
43	RO	122	933	588	171	170	4	0	0	0
43	YO	122	933	588	171	170	4	0	0	0

- Molecule 44 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
44	RP	150	1145	712	232	198	3	0	0	0
44	YP	150	1145	712	232	198	3	0	0	0

- Molecule 45 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
45	RQ	141	1122	715	212	188	7	0	0	0
45	YQ	141	1122	715	212	188	7	0	0	0

- Molecule 46 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
46	RR	118	968	604	203	160	1	0	0	0
46	YR	118	968	604	203	160	1	0	0	0

- Molecule 47 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
47	RS	111	882	556	176	150	0	0	0
47	YS	111	882	556	176	150	0	0	0

- Molecule 48 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
48	RT	137	Total 1141	C 710	N 234	O 196	S 1	0	0	0
48	YT	137	Total 1141	C 710	N 234	O 196	S 1	0	0	0

- Molecule 49 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
49	RU	117	Total 964	C 610	N 202	O 151	S 1	0	0	0
49	YU	117	Total 964	C 610	N 202	O 151	S 1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
50	RV	101	Total 779	C 501	N 142	O 135	S 1	0	0	0
50	YV	101	Total 779	C 501	N 142	O 135	S 1	0	0	0

- Molecule 51 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
51	RW	113	Total 900	C 566	N 177	O 155	S 2	0	0	0
51	YW	113	Total 900	C 566	N 177	O 155	S 2	0	0	0

- Molecule 52 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
52	RX	92	Total 725	C 471	N 131	O 123	0	0	0
52	YX	92	Total 725	C 471	N 131	O 123	0	0	0

- Molecule 53 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	RY	102	Total	C	N	O	S	0	0	0
			785	505	150	125	5			
53	YY	102	Total	C	N	O	S	0	0	0
			785	505	150	125	5			

- Molecule 54 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	RZ	183	Total	C	N	O	S	0	0	0
			1461	933	260	265	3			
54	YZ	183	Total	C	N	O	S	0	0	0
			1461	933	260	265	3			

- Molecule 55 is a RNA chain called A-site ASL[^]Phe.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	XY	17	Total	C	N	O	P	0	0	0
			362	163	68	115	16			

- Molecule 56 is a RNA chain called CC-puro.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	Z6	3	Total	C	N	O	P	0	0	0
			74	40	13	19	2			
56	Z8	3	Total	C	N	O	P	0	0	0
			74	40	13	19	2			

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

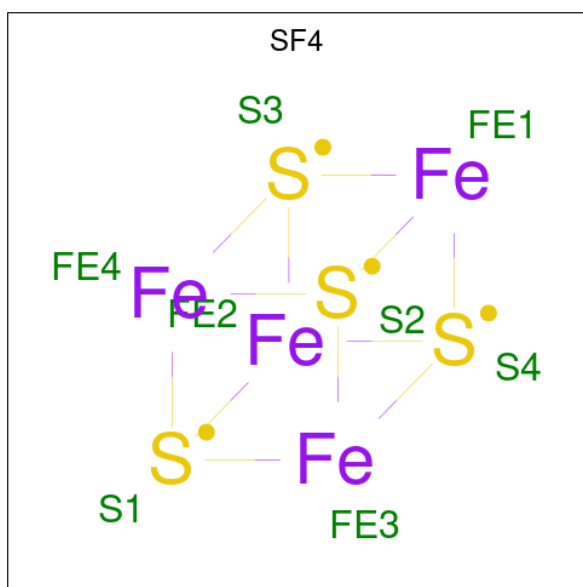
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QA	54	Total	Mg	0	0
			54	54		
57	QV	1	Total	Mg	0	0
			1	1		
57	R0	1	Total	Mg	0	0
			1	1		
57	R5	1	Total	Mg	0	0
			1	1		
57	R7	1	Total	Mg	0	0
			1	1		
57	R8	1	Total	Mg	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	RA	333	Total 333	Mg 333	0	0
57	RB	5	Total 5	Mg 5	0	0
57	RE	1	Total 1	Mg 1	0	0
57	RF	1	Total 1	Mg 1	0	0
57	RR	2	Total 2	Mg 2	0	0
57	XA	58	Total 58	Mg 58	0	0
57	XV	2	Total 2	Mg 2	0	0
57	XX	1	Total 1	Mg 1	0	0
57	Y0	1	Total 1	Mg 1	0	0
57	Y1	1	Total 1	Mg 1	0	0
57	Y3	1	Total 1	Mg 1	0	0
57	Y5	1	Total 1	Mg 1	0	0
57	Y7	2	Total 2	Mg 2	0	0
57	YA	361	Total 361	Mg 361	0	0
57	YB	4	Total 4	Mg 4	0	0
57	YE	2	Total 2	Mg 2	0	0
57	YP	2	Total 2	Mg 2	0	0
57	YQ	2	Total 2	Mg 2	0	0
57	YR	2	Total 2	Mg 2	0	0
57	YY	1	Total 1	Mg 1	0	0

- Molecule 58 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	QD	1	Total	Fe S	0	0
			8	4 4		
58	XD	1	Total	Fe S	0	0
			8	4 4		

- Molecule 59 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	QN	1	Total	Zn	0	0
			1	1		
59	XN	1	Total	Zn	0	0
			1	1		

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	209.72Å 449.48Å 617.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	153.33 – 3.58 153.33 – 3.58	Depositor EDS
% Data completeness (in resolution range)	98.3 (153.33-3.58) 98.3 (153.33-3.58)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 3.41Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.205 , 0.255 0.205 , 0.254	Depositor DCC
R_{free} test set	35613 reflections (4.51%)	wwPDB-VP
Wilson B-factor (Å ²)	96.7	Xtrriage
Anisotropy	0.201	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 132.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	292176	wwPDB-VP
Average B, all atoms (Å ²)	118.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.75% 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](#)

18 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
22	T6A	XV	37	22	31,34,35	1.39	4 (12%)	43,49,52	1.88	12 (27%)
22	PSU	QV	39	22	18,21,22	1.41	2 (11%)	21,30,33	2.10	4 (19%)
22	C4J	QV	47	22	25,29,30	2.87	7 (28%)	28,42,45	1.74	5 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	H2U	QV	20	22	18,21,22	1.04	1 (5%)	19,30,33	1.36	3 (15%)
22	MNU	XV	34	22,23	21,24,25	1.25	4 (19%)	27,34,37	1.84	7 (25%)
22	7MG	QV	46	22	23,26,27	1.39	5 (21%)	27,39,42	2.52	5 (18%)
22	MNU	QV	34	22,23	21,24,25	1.24	3 (14%)	27,34,37	1.71	8 (29%)
22	H2U	XV	20	22	18,21,22	1.04	2 (11%)	19,30,33	1.23	3 (15%)
22	5MU	QV	54	22	19,22,23	1.36	4 (21%)	27,32,35	2.07	8 (29%)
22	PSU	XV	55	22	18,21,22	1.39	2 (11%)	21,30,33	2.02	3 (14%)
22	5MU	XV	54	22	19,22,23	1.36	5 (26%)	27,32,35	2.01	7 (25%)
56	PPU	Z6	76	56,34	37,40,41	1.28	4 (10%)	47,57,60	2.03	12 (25%)
56	PPU	Z8	76	56,34	37,40,41	1.32	4 (10%)	47,57,60	2.02	12 (25%)
22	PSU	XV	39	22	18,21,22	1.39	2 (11%)	21,30,33	1.99	3 (14%)
22	7MG	XV	46	22	23,26,27	1.30	3 (13%)	27,39,42	2.62	7 (25%)
22	T6A	QV	37	22	31,34,35	1.37	4 (12%)	43,49,52	2.04	12 (27%)
22	PSU	QV	55	22	18,21,22	1.44	2 (11%)	21,30,33	2.09	4 (19%)
22	C4J	XV	47	22	25,29,30	2.79	6 (24%)	28,42,45	1.57	5 (17%)

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
22	T6A	XV	37	22	-	8/23/41/42	0/3/3/3
22	PSU	QV	39	22	-	0/7/25/26	0/2/2/2
22	C4J	QV	47	22	-	4/16/34/35	0/2/2/2
22	H2U	QV	20	22	-	5/7/38/39	0/2/2/2
22	MNU	XV	34	22,23	-	4/10/28/29	0/2/2/2
22	7MG	QV	46	22	-	2/7/37/38	0/3/3/3
22	MNU	QV	34	22,23	-	2/10/28/29	0/2/2/2
22	H2U	XV	20	22	-	5/7/38/39	0/2/2/2
22	5MU	QV	54	22	-	0/7/25/26	0/2/2/2
22	PSU	XV	55	22	-	0/7/25/26	0/2/2/2
22	5MU	XV	54	22	-	0/7/25/26	0/2/2/2
56	PPU	Z6	76	56,34	-	3/25/43/44	0/4/4/4
56	PPU	Z8	76	56,34	-	3/25/43/44	0/4/4/4
22	PSU	XV	39	22	-	0/7/25/26	0/2/2/2
22	7MG	XV	46	22	-	0/7/37/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	T6A	QV	37	22	-	10/23/41/42	0/3/3/3
22	PSU	QV	55	22	-	0/7/25/26	0/2/2/2
22	C4J	XV	47	22	-	4/16/34/35	0/2/2/2

The worst 5 of 64 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	QV	47	C4J	C6-C5	10.37	1.49	1.35
22	XV	47	C4J	C6-C5	10.21	1.49	1.35
22	QV	47	C4J	C2-N3	6.56	1.50	1.38
22	XV	47	C4J	C2-N3	6.10	1.49	1.38
56	Z8	76	PPU	C5-C4	5.15	1.48	1.39

The worst 5 of 120 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	XV	46	7MG	N9-C4-N3	8.91	138.52	125.46
22	QV	46	7MG	N9-C4-N3	8.70	138.21	125.46
22	QV	55	PSU	N1-C2-N3	6.73	122.27	115.17
22	QV	39	PSU	N1-C2-N3	6.33	121.84	115.17
22	XV	55	PSU	N1-C2-N3	6.19	121.70	115.17

There are no chirality outliers.

5 of 50 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	XV	20	H2U	C2'-C1'-N1-C2
22	QV	34	MNU	C6-C5-C7-N8
22	QV	34	MNU	C4-C5-C7-N8
22	XV	34	MNU	C6-C5-C7-N8
22	XV	34	MNU	C4-C5-C7-N8

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 846 ligands modelled in this entry, 844 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
58	SF4	XD	301	4	0,12,12	-	-	-		
58	SF4	QD	301	4	0,12,12	-	-	-		

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
58	SF4	XD	301	4	-	-	0/6/5/5
58	SF4	QD	301	4	-	-	0/6/5/5

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 [i](#)

5.1 Protein, DNA and RNA chains [i](#)

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	QA	1500/1522 (98%)	-0.02	15 (1%) 79 53	65, 123, 231, 395	0
1	XA	1511/1522 (99%)	0.08	57 (3%) 44 24	60, 122, 218, 363	0
2	QB	237/256 (92%)	0.21	3 (1%) 75 47	122, 192, 248, 311	0
2	XB	237/256 (92%)	0.26	3 (1%) 75 47	90, 152, 222, 280	0
3	QC	205/239 (85%)	-0.01	3 (1%) 72 44	95, 174, 232, 279	0
3	XC	205/239 (85%)	-0.06	1 (0%) 87 66	93, 142, 199, 231	0
4	QD	208/209 (99%)	0.43	5 (2%) 59 34	97, 139, 197, 245	0
4	XD	208/209 (99%)	0.19	1 (0%) 87 66	68, 116, 161, 186	0
5	QE	151/162 (93%)	0.24	2 (1%) 75 47	95, 143, 186, 218	0
5	XE	151/162 (93%)	-0.05	1 (0%) 84 60	68, 108, 150, 194	0
6	QF	101/101 (100%)	0.27	1 (0%) 79 53	83, 130, 181, 207	0
6	XF	101/101 (100%)	0.53	3 (2%) 52 29	74, 120, 168, 261	0
7	QG	155/156 (99%)	0.49	11 (7%) 22 13	118, 166, 226, 275	0
7	XG	155/156 (99%)	0.26	6 (3%) 43 23	103, 152, 208, 237	0
8	QH	138/138 (100%)	0.16	2 (1%) 73 45	95, 138, 183, 215	0
8	XH	138/138 (100%)	0.34	6 (4%) 40 21	76, 125, 172, 207	0
9	QI	127/128 (99%)	0.39	5 (3%) 43 23	129, 184, 234, 307	0
9	XI	127/128 (99%)	0.36	12 (9%) 14 9	107, 164, 221, 281	0
10	QJ	99/105 (94%)	0.41	1 (1%) 79 53	136, 190, 252, 301	0
10	XJ	99/105 (94%)	0.32	3 (3%) 52 29	110, 166, 215, 265	0
11	QK	119/129 (92%)	0.42	7 (5%) 28 16	98, 129, 188, 255	0
11	XK	119/129 (92%)	0.38	4 (3%) 48 27	73, 117, 190, 277	0
12	QL	125/131 (95%)	0.35	6 (4%) 35 19	74, 111, 159, 237	0
12	XL	125/131 (95%)	0.20	4 (3%) 50 28	57, 98, 155, 256	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	QM	121/126 (96%)	0.77	13 (10%) 11 8	123, 171, 219, 278	0
13	XM	121/126 (96%)	0.32	6 (4%) 34 19	103, 159, 199, 257	0
14	QN	60/61 (98%)	0.14	0 100 100	122, 169, 222, 250	0
14	XN	60/61 (98%)	0.28	3 (5%) 34 19	103, 138, 172, 195	0
15	QO	88/89 (98%)	0.50	6 (6%) 23 14	75, 124, 170, 188	0
15	XO	88/89 (98%)	0.47	5 (5%) 29 17	71, 109, 157, 184	0
16	QP	84/88 (95%)	0.51	4 (4%) 35 19	76, 108, 155, 224	0
16	XP	84/88 (95%)	0.21	1 (1%) 76 49	92, 131, 184, 200	0
17	QQ	100/105 (95%)	0.36	3 (3%) 52 29	81, 114, 149, 170	0
17	XQ	100/105 (95%)	0.38	2 (2%) 65 37	84, 123, 166, 173	0
18	QR	70/88 (79%)	-0.04	1 (1%) 73 45	100, 140, 181, 188	0
18	XR	70/88 (79%)	0.38	0 100 100	81, 120, 160, 191	0
19	QS	84/93 (90%)	0.12	0 100 100	134, 188, 256, 354	0
19	XS	84/93 (90%)	0.12	3 (3%) 46 25	127, 176, 238, 259	0
20	QT	99/106 (93%)	0.46	6 (6%) 27 15	72, 110, 169, 235	0
20	XT	99/106 (93%)	0.28	3 (3%) 52 29	107, 146, 209, 231	0
21	QU	25/27 (92%)	1.43	5 (20%) 3 3	145, 175, 223, 226	0
21	XU	25/27 (92%)	0.20	0 100 100	125, 154, 200, 213	0
22	QV	66/76 (86%)	0.70	6 (9%) 15 10	124, 253, 275, 293	0
22	XV	66/76 (86%)	0.44	6 (9%) 15 10	102, 217, 247, 262	0
23	QX	3/23 (13%)	0.37	0 100 100	99, 99, 100, 127	0
23	XX	23/23 (100%)	1.72	7 (30%) 1 1	97, 220, 268, 305	0
24	R0	82/85 (96%)	0.34	3 (3%) 45 25	68, 103, 148, 184	0
24	Y0	82/85 (96%)	0.44	4 (4%) 35 19	63, 105, 132, 169	0
25	R1	97/98 (98%)	0.65	8 (8%) 17 11	38, 92, 165, 221	0
25	Y1	97/98 (98%)	0.41	5 (5%) 33 18	54, 84, 170, 254	0
26	R2	69/72 (95%)	0.15	0 100 100	71, 116, 170, 206	0
26	Y2	71/72 (98%)	0.17	2 (2%) 55 30	56, 88, 160, 261	0
27	R3	59/60 (98%)	0.31	1 (1%) 69 40	69, 99, 170, 231	0
27	Y3	59/60 (98%)	0.20	2 (3%) 48 27	73, 100, 152, 177	0
28	R4	71/71 (100%)	0.24	0 100 100	150, 221, 299, 329	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	Y4	71/71 (100%)	0.26	2 (2%) 55 30	125, 199, 313, 339	0
29	R5	59/60 (98%)	0.39	4 (6%) 23 14	53, 89, 208, 249	0
29	Y5	59/60 (98%)	0.46	4 (6%) 23 14	60, 92, 216, 310	0
30	R6	49/54 (90%)	0.84	5 (10%) 12 8	191, 247, 316, 341	0
30	Y6	49/54 (90%)	0.59	2 (4%) 41 22	179, 236, 296, 337	0
31	R7	49/49 (100%)	-0.01	0 100 100	43, 62, 136, 244	0
31	Y7	49/49 (100%)	0.15	2 (4%) 41 22	44, 60, 138, 178	0
32	R8	64/65 (98%)	0.62	7 (10%) 10 8	54, 88, 134, 328	0
32	Y8	64/65 (98%)	0.98	10 (15%) 5 5	67, 92, 166, 199	0
33	R9	37/37 (100%)	1.82	15 (40%) 0 1	152, 211, 269, 297	0
33	Y9	37/37 (100%)	2.11	18 (48%) 0 1	178, 217, 280, 312	0
34	RA	2882/2915 (98%)	-0.19	17 (0%) 85 63	43, 83, 229, 398	0
34	YA	2883/2915 (98%)	-0.11	34 (1%) 76 49	41, 82, 243, 435	0
35	RB	120/122 (98%)	0.09	0 100 100	96, 165, 199, 259	0
35	YB	120/122 (98%)	-0.02	1 (0%) 82 58	94, 134, 169, 250	0
36	RD	272/276 (98%)	0.39	10 (3%) 45 25	43, 78, 113, 165	0
36	YD	272/276 (98%)	0.34	11 (4%) 42 23	38, 72, 110, 221	0
37	RE	205/206 (99%)	0.13	3 (1%) 72 44	45, 81, 146, 270	0
37	YE	205/206 (99%)	0.32	5 (2%) 59 34	46, 98, 154, 210	0
38	RF	202/210 (96%)	0.34	9 (4%) 38 20	50, 92, 160, 191	0
38	YF	202/210 (96%)	0.05	1 (0%) 87 66	39, 84, 141, 190	0
39	RG	181/182 (99%)	0.35	4 (2%) 62 35	132, 183, 256, 304	0
39	YG	181/182 (99%)	0.38	3 (1%) 69 40	102, 147, 200, 251	0
40	RH	170/180 (94%)	0.57	13 (7%) 20 12	79, 170, 240, 274	0
40	YH	170/180 (94%)	0.44	10 (5%) 28 16	70, 111, 159, 274	0
41	RI	146/148 (98%)	0.44	7 (4%) 35 19	74, 130, 184, 350	0
41	YI	146/148 (98%)	0.24	4 (2%) 56 31	68, 123, 187, 214	0
42	RN	138/140 (98%)	0.35	2 (1%) 73 45	66, 97, 153, 213	0
42	YN	138/140 (98%)	0.18	2 (1%) 73 45	58, 100, 155, 209	0
43	RO	122/122 (100%)	0.04	2 (1%) 70 42	40, 75, 113, 136	0
43	YO	122/122 (100%)	-0.02	0 100 100	48, 83, 123, 145	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	RP	150/150 (100%)	0.30	7 (4%) 36 19	53, 105, 160, 276	0
44	YP	150/150 (100%)	0.61	9 (6%) 27 16	50, 101, 167, 244	0
45	RQ	141/141 (100%)	0.49	9 (6%) 25 15	67, 103, 157, 208	0
45	YQ	141/141 (100%)	0.57	15 (10%) 11 8	58, 99, 159, 242	0
46	RR	118/118 (100%)	0.02	1 (0%) 82 58	45, 74, 104, 157	0
46	YR	118/118 (100%)	0.18	4 (3%) 48 27	59, 90, 135, 188	0
47	RS	111/112 (99%)	0.25	2 (1%) 67 40	119, 147, 209, 253	0
47	YS	111/112 (99%)	0.55	2 (1%) 67 40	88, 138, 185, 278	0
48	RT	137/146 (93%)	0.34	6 (4%) 39 21	52, 91, 157, 192	0
48	YT	137/146 (93%)	0.14	1 (0%) 84 60	67, 101, 174, 238	0
49	RU	117/118 (99%)	0.29	4 (3%) 48 27	51, 90, 156, 186	0
49	YU	117/118 (99%)	0.19	3 (2%) 57 32	54, 91, 152, 204	0
50	RV	101/101 (100%)	0.31	4 (3%) 42 23	63, 110, 150, 242	0
50	YV	101/101 (100%)	0.23	2 (1%) 65 37	64, 111, 165, 252	0
51	RW	113/113 (100%)	0.01	2 (1%) 67 40	48, 71, 131, 285	0
51	YW	113/113 (100%)	-0.00	1 (0%) 81 55	43, 76, 144, 212	0
52	RX	92/96 (95%)	0.05	1 (1%) 78 51	64, 90, 128, 173	0
52	YX	92/96 (95%)	-0.17	0 100 100	45, 74, 112, 148	0
53	RY	102/110 (92%)	0.89	12 (11%) 9 7	69, 115, 172, 303	0
53	YY	102/110 (92%)	0.57	6 (5%) 28 16	52, 98, 178, 233	0
54	RZ	183/206 (88%)	0.21	4 (2%) 62 35	90, 142, 188, 229	0
54	YZ	183/206 (88%)	0.40	10 (5%) 30 17	94, 136, 200, 254	0
55	XY	17/17 (100%)	0.21	0 100 100	133, 179, 250, 263	0
56	Z6	2/3 (66%)	0.51	0 100 100	148, 148, 148, 152	0
56	Z8	2/3 (66%)	1.01	0 100 100	156, 156, 156, 156	0
All	All	20863/21465 (97%)	0.15	579 (2%) 55 30	38, 111, 222, 435	0

The worst 5 of 579 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	QM	120	LYS	9.3
11	XK	129	SER	7.4
7	XG	5	ARG	7.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
11	XK	128	ALA	7.3
34	YA	669	G	6.3

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
22	C4J	QV	47	28/29	0.19	0.16	216,236,255,258	0
22	C4J	XV	47	28/29	0.26	0.14	216,238,248,253	0
22	H2U	QV	20	20/21	0.33	0.12	350,356,363,365	0
22	7MG	QV	46	24/25	0.55	0.10	269,282,291,313	0
22	5MU	XV	54	21/22	0.67	0.10	220,226,234,237	0
22	H2U	XV	20	20/21	0.72	0.09	264,273,283,285	0
22	PSU	XV	55	20/21	0.72	0.08	225,233,240,242	0
22	5MU	QV	54	21/22	0.73	0.09	229,235,242,243	0
22	7MG	XV	46	24/25	0.76	0.08	214,229,235,237	0
22	PSU	QV	55	20/21	0.77	0.09	234,239,249,252	0
22	T6A	QV	37	32/33	0.77	0.17	138,161,200,207	0
22	T6A	XV	37	32/33	0.88	0.14	96,111,152,158	0
22	PSU	QV	39	20/21	0.89	0.10	122,123,132,138	0
22	MNU	XV	34	23/24	0.92	0.11	95,100,117,132	0
22	PSU	XV	39	20/21	0.93	0.10	91,100,120,125	0
22	MNU	QV	34	23/24	0.94	0.10	121,122,145,148	0
56	PPU	Z8	76	37/38	0.95	0.13	74,104,122,130	0
56	PPU	Z6	76	37/38	0.96	0.12	76,109,123,127	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(\AA^2)	Q<0.9
57	MG	Y7	102	1/1	-0.08	0.21	72,72,72,72	0
57	MG	YA	3265	1/1	0.20	0.18	254,254,254,254	0
57	MG	YA	3300	1/1	0.26	0.46	109,109,109,109	0
57	MG	YA	3359	1/1	0.30	0.20	78,78,78,78	0
57	MG	RB	202	1/1	0.33	0.10	129,129,129,129	0
57	MG	YA	3184	1/1	0.40	0.22	190,190,190,190	0
57	MG	YA	3339	1/1	0.43	0.30	132,132,132,132	0
57	MG	RA	3224	1/1	0.43	0.22	110,110,110,110	0
57	MG	QA	1642	1/1	0.46	0.27	111,111,111,111	0
57	MG	YA	3315	1/1	0.46	0.33	151,151,151,151	0
57	MG	YA	3223	1/1	0.47	0.15	71,71,71,71	0
57	MG	RA	3129	1/1	0.50	0.19	92,92,92,92	0
57	MG	RA	3203	1/1	0.53	0.25	84,84,84,84	0
57	MG	YA	3323	1/1	0.55	0.20	94,94,94,94	0
57	MG	YA	3341	1/1	0.56	0.28	122,122,122,122	0
57	MG	YA	3152	1/1	0.57	0.11	99,99,99,99	0
57	MG	RA	3209	1/1	0.59	0.14	76,76,76,76	0
57	MG	YA	3358	1/1	0.61	0.45	140,140,140,140	0
57	MG	YA	3171	1/1	0.62	0.12	136,136,136,136	0
57	MG	YA	3349	1/1	0.63	0.15	72,72,72,72	0
57	MG	YA	3354	1/1	0.63	0.19	76,76,76,76	0
57	MG	QA	1646	1/1	0.63	0.16	97,97,97,97	0
57	MG	YA	3335	1/1	0.63	0.36	129,129,129,129	0
57	MG	YA	3221	1/1	0.64	0.13	54,54,54,54	0
57	MG	YA	3340	1/1	0.65	0.08	62,62,62,62	0
57	MG	RA	3261	1/1	0.67	0.20	84,84,84,84	0
57	MG	XA	1639	1/1	0.67	0.11	138,138,138,138	0
57	MG	YR	201	1/1	0.67	0.12	81,81,81,81	0
57	MG	QA	1645	1/1	0.68	0.16	98,98,98,98	0
57	MG	Y0	101	1/1	0.69	0.22	80,80,80,80	0
57	MG	YA	3307	1/1	0.70	0.29	76,76,76,76	0
57	MG	XA	1650	1/1	0.70	0.17	65,65,65,65	0
57	MG	YA	3186	1/1	0.70	0.21	73,73,73,73	0
57	MG	RA	3149	1/1	0.71	0.12	64,64,64,64	0
57	MG	RA	3001	1/1	0.71	0.37	134,134,134,134	0
57	MG	RA	3283	1/1	0.72	0.16	65,65,65,65	0
57	MG	YA	3322	1/1	0.72	0.13	84,84,84,84	0
57	MG	YE	301	1/1	0.72	0.16	38,38,38,38	0
57	MG	YA	3266	1/1	0.72	0.14	82,82,82,82	0
57	MG	QA	1635	1/1	0.73	0.13	101,101,101,101	0
57	MG	YA	3135	1/1	0.73	0.12	51,51,51,51	0
57	MG	YA	3350	1/1	0.73	0.16	83,83,83,83	0
57	MG	YA	3214	1/1	0.73	0.17	40,40,40,40	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	MG	YA	3344	1/1	0.74	0.20	92,92,92,92	0
57	MG	RA	3165	1/1	0.74	0.10	61,61,61,61	0
57	MG	YB	204	1/1	0.74	0.27	67,67,67,67	0
57	MG	YA	3115	1/1	0.74	0.14	88,88,88,88	0
57	MG	YA	3336	1/1	0.74	0.33	72,72,72,72	0
57	MG	XA	1654	1/1	0.75	0.15	97,97,97,97	0
57	MG	YA	3326	1/1	0.76	0.10	73,73,73,73	0
57	MG	YA	3288	1/1	0.76	0.11	112,112,112,112	0
57	MG	YA	3211	1/1	0.76	0.18	90,90,90,90	0
57	MG	YA	3181	1/1	0.77	0.12	82,82,82,82	0
57	MG	YA	3151	1/1	0.77	0.20	62,62,62,62	0
57	MG	RA	3277	1/1	0.77	0.21	54,54,54,54	0
57	MG	YA	3191	1/1	0.77	0.31	85,85,85,85	0
57	MG	YA	3282	1/1	0.77	0.26	111,111,111,111	0
57	MG	YA	3204	1/1	0.77	0.14	66,66,66,66	0
57	MG	YA	3166	1/1	0.77	0.13	79,79,79,79	0
57	MG	YA	3301	1/1	0.77	0.09	39,39,39,39	0
57	MG	RA	3274	1/1	0.77	0.17	94,94,94,94	0
57	MG	XA	1649	1/1	0.78	0.31	83,83,83,83	0
57	MG	QA	1638	1/1	0.78	0.18	104,104,104,104	0
57	MG	YB	201	1/1	0.78	0.17	47,47,47,47	0
57	MG	YA	3261	1/1	0.79	0.13	55,55,55,55	0
57	MG	YA	3263	1/1	0.79	0.33	76,76,76,76	0
57	MG	XA	1613	1/1	0.79	0.24	50,50,50,50	0
57	MG	YA	3213	1/1	0.79	0.18	79,79,79,79	0
57	MG	YA	3187	1/1	0.79	0.22	59,59,59,59	0
57	MG	RA	3326	1/1	0.79	0.09	17,17,17,17	0
57	MG	RA	3250	1/1	0.79	0.11	34,34,34,34	0
57	MG	YA	3264	1/1	0.80	0.16	91,91,91,91	0
57	MG	QA	1611	1/1	0.80	0.12	66,66,66,66	0
57	MG	YA	3338	1/1	0.80	0.15	86,86,86,86	0
57	MG	RA	3273	1/1	0.80	0.12	40,40,40,40	0
57	MG	YA	3318	1/1	0.80	0.28	120,120,120,120	0
57	MG	YA	3244	1/1	0.80	0.21	31,31,31,31	0
57	MG	XA	1622	1/1	0.80	0.14	63,63,63,63	0
57	MG	RA	3190	1/1	0.80	0.29	52,52,52,52	0
57	MG	YA	3168	1/1	0.81	0.08	70,70,70,70	0
57	MG	YA	3142	1/1	0.81	0.24	52,52,52,52	0
57	MG	RA	3010	1/1	0.81	0.12	59,59,59,59	0
57	MG	YA	3360	1/1	0.81	0.17	100,100,100,100	0
57	MG	YA	3294	1/1	0.81	0.12	63,63,63,63	0
57	MG	QA	1641	1/1	0.81	0.11	104,104,104,104	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	YA	3157	1/1	0.81	0.12	49,49,49,49	0
57	MG	RA	3246	1/1	0.81	0.17	77,77,77,77	0
57	MG	YA	3328	1/1	0.82	0.14	39,39,39,39	0
57	MG	YA	3216	1/1	0.82	0.27	85,85,85,85	0
57	MG	RA	3286	1/1	0.82	0.20	55,55,55,55	0
57	MG	RA	3211	1/1	0.82	0.16	76,76,76,76	0
57	MG	YA	3324	1/1	0.82	0.22	87,87,87,87	0
57	MG	YQ	202	1/1	0.82	0.12	88,88,88,88	0
57	MG	XA	1652	1/1	0.82	0.09	54,54,54,54	0
57	MG	YA	3331	1/1	0.83	0.07	53,53,53,53	0
57	MG	YA	3343	1/1	0.83	0.13	96,96,96,96	0
57	MG	RA	3310	1/1	0.83	0.22	76,76,76,76	0
57	MG	YA	3279	1/1	0.83	0.10	56,56,56,56	0
57	MG	XA	1614	1/1	0.83	0.11	53,53,53,53	0
57	MG	RA	3196	1/1	0.83	0.11	67,67,67,67	0
57	MG	RA	3299	1/1	0.83	0.14	68,68,68,68	0
57	MG	YA	3332	1/1	0.84	0.09	56,56,56,56	0
57	MG	YA	3190	1/1	0.84	0.11	84,84,84,84	0
57	MG	Y1	101	1/1	0.84	0.19	91,91,91,91	0
57	MG	YA	3319	1/1	0.84	0.28	63,63,63,63	0
57	MG	YA	3175	1/1	0.84	0.23	94,94,94,94	0
57	MG	YA	3257	1/1	0.84	0.17	36,36,36,36	0
57	MG	RA	3201	1/1	0.84	0.17	70,70,70,70	0
57	MG	RA	3291	1/1	0.84	0.27	37,37,37,37	0
57	MG	RA	3120	1/1	0.84	0.18	47,47,47,47	0
57	MG	RA	3303	1/1	0.84	0.07	92,92,92,92	0
57	MG	QA	1639	1/1	0.85	0.11	88,88,88,88	0
57	MG	RA	3248	1/1	0.85	0.11	33,33,33,33	0
57	MG	YA	3120	1/1	0.85	0.12	39,39,39,39	0
57	MG	YA	3345	1/1	0.85	0.14	83,83,83,83	0
57	MG	YA	3348	1/1	0.85	0.19	83,83,83,83	0
57	MG	YA	3124	1/1	0.85	0.09	56,56,56,56	0
57	MG	RA	3215	1/1	0.85	0.14	59,59,59,59	0
57	MG	RA	3210	1/1	0.85	0.20	63,63,63,63	0
57	MG	YA	3231	1/1	0.85	0.08	53,53,53,53	0
57	MG	YA	3296	1/1	0.85	0.17	47,47,47,47	0
57	MG	YA	3298	1/1	0.85	0.19	126,126,126,126	0
57	MG	RB	203	1/1	0.85	0.22	29,29,29,29	0
57	MG	RB	205	1/1	0.85	0.19	58,58,58,58	0
57	MG	YA	3302	1/1	0.85	0.16	76,76,76,76	0
57	MG	RA	3270	1/1	0.85	0.17	46,46,46,46	0
57	MG	RA	3226	1/1	0.85	0.34	75,75,75,75	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	RA	3131	1/1	0.86	0.27	39,39,39,39	0
57	MG	YA	3136	1/1	0.86	0.15	72,72,72,72	0
57	MG	QA	1619	1/1	0.86	0.07	63,63,63,63	0
57	MG	YA	3193	1/1	0.86	0.18	95,95,95,95	0
57	MG	YA	3281	1/1	0.86	0.24	84,84,84,84	0
57	MG	RA	3012	1/1	0.86	0.12	17,17,17,17	0
57	MG	RA	3170	1/1	0.86	0.11	71,71,71,71	0
57	MG	XA	1643	1/1	0.86	0.06	56,56,56,56	0
57	MG	YA	3162	1/1	0.86	0.17	56,56,56,56	0
57	MG	RA	3053	1/1	0.87	0.24	31,31,31,31	0
57	MG	XA	1604	1/1	0.87	0.10	56,56,56,56	0
57	MG	YA	3205	1/1	0.87	0.19	104,104,104,104	0
57	MG	RA	3009	1/1	0.87	0.23	75,75,75,75	0
57	MG	RA	3267	1/1	0.87	0.09	60,60,60,60	0
57	MG	YA	3295	1/1	0.87	0.16	31,31,31,31	0
57	MG	YA	3106	1/1	0.87	0.17	156,156,156,156	0
57	MG	QA	1630	1/1	0.87	0.20	72,72,72,72	0
57	MG	YA	3299	1/1	0.87	0.19	73,73,73,73	0
57	MG	YA	3218	1/1	0.87	0.17	67,67,67,67	0
57	MG	YA	3169	1/1	0.87	0.11	17,17,17,17	0
57	MG	YA	3170	1/1	0.87	0.11	86,86,86,86	0
57	MG	RA	3003	1/1	0.87	0.10	34,34,34,34	0
57	MG	YA	3121	1/1	0.87	0.24	44,44,44,44	0
57	MG	YA	3123	1/1	0.87	0.33	45,45,45,45	0
57	MG	YA	3260	1/1	0.87	0.08	85,85,85,85	0
57	MG	RA	3138	1/1	0.87	0.17	47,47,47,47	0
57	MG	RA	3333	1/1	0.87	0.23	55,55,55,55	0
57	MG	RA	3014	1/1	0.87	0.29	30,30,30,30	0
57	MG	RA	3154	1/1	0.87	0.12	94,94,94,94	0
57	MG	YA	3146	1/1	0.87	0.11	66,66,66,66	0
57	MG	YA	3268	1/1	0.87	0.22	42,42,42,42	0
57	MG	YR	202	1/1	0.87	0.30	82,82,82,82	0
57	MG	YA	3161	1/1	0.88	0.28	47,47,47,47	0
57	MG	RA	3315	1/1	0.88	0.14	48,48,48,48	0
57	MG	YA	3164	1/1	0.88	0.24	47,47,47,47	0
57	MG	RA	3322	1/1	0.88	0.09	68,68,68,68	0
57	MG	YA	3247	1/1	0.88	0.23	81,81,81,81	0
57	MG	YA	3252	1/1	0.88	0.12	139,139,139,139	0
57	MG	RA	3200	1/1	0.88	0.12	74,74,74,74	0
57	MG	RA	3130	1/1	0.88	0.26	52,52,52,52	0
57	MG	RA	3163	1/1	0.88	0.18	28,28,28,28	0
57	MG	YA	3070	1/1	0.88	0.12	19,19,19,19	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	YA	3083	1/1	0.88	0.18	68,68,68,68	0
57	MG	YA	3105	1/1	0.88	0.25	38,38,38,38	0
57	MG	YA	3182	1/1	0.88	0.11	56,56,56,56	0
57	MG	RA	3011	1/1	0.88	0.15	92,92,92,92	0
57	MG	RA	3124	1/1	0.88	0.24	28,28,28,28	0
57	MG	RR	202	1/1	0.88	0.22	62,62,62,62	0
57	MG	XA	1603	1/1	0.88	0.13	63,63,63,63	0
57	MG	RA	3290	1/1	0.88	0.16	69,69,69,69	0
57	MG	YA	3291	1/1	0.88	0.10	47,47,47,47	0
57	MG	RA	3251	1/1	0.88	0.26	53,53,53,53	0
57	MG	YA	3202	1/1	0.88	0.06	52,52,52,52	0
57	MG	RA	3296	1/1	0.88	0.18	55,55,55,55	0
57	MG	QA	1621	1/1	0.88	0.19	67,67,67,67	0
57	MG	YA	3210	1/1	0.88	0.12	87,87,87,87	0
57	MG	RA	3153	1/1	0.88	0.23	45,45,45,45	0
57	MG	YA	3212	1/1	0.88	0.11	126,126,126,126	0
57	MG	RA	3307	1/1	0.88	0.14	60,60,60,60	0
57	MG	YP	201	1/1	0.88	0.31	89,89,89,89	0
57	MG	XA	1647	1/1	0.88	0.19	39,39,39,39	0
57	MG	RA	3220	1/1	0.88	0.15	53,53,53,53	0
57	MG	RA	3312	1/1	0.88	0.11	49,49,49,49	0
57	MG	YA	3287	1/1	0.89	0.09	32,32,32,32	0
57	MG	YA	3178	1/1	0.89	0.10	69,69,69,69	0
57	MG	YA	3290	1/1	0.89	0.15	88,88,88,88	0
57	MG	YA	3180	1/1	0.89	0.16	81,81,81,81	0
57	MG	YA	3292	1/1	0.89	0.28	85,85,85,85	0
57	MG	YA	3220	1/1	0.89	0.17	68,68,68,68	0
57	MG	YA	3139	1/1	0.89	0.19	92,92,92,92	0
57	MG	RA	3281	1/1	0.89	0.15	46,46,46,46	0
57	MG	Y7	101	1/1	0.89	0.15	55,55,55,55	0
57	MG	XA	1625	1/1	0.89	0.13	59,59,59,59	0
57	MG	XA	1627	1/1	0.89	0.19	43,43,43,43	0
57	MG	RA	3171	1/1	0.89	0.17	62,62,62,62	0
57	MG	RB	204	1/1	0.89	0.34	58,58,58,58	0
57	MG	XA	1644	1/1	0.89	0.06	65,65,65,65	0
57	MG	RA	3186	1/1	0.89	0.23	60,60,60,60	0
57	MG	YA	3203	1/1	0.89	0.12	64,64,64,64	0
57	MG	RA	3070	1/1	0.89	0.16	28,28,28,28	0
57	MG	YA	3361	1/1	0.89	0.14	41,41,41,41	0
57	MG	RA	3249	1/1	0.89	0.26	116,116,116,116	0
57	MG	YB	202	1/1	0.89	0.24	199,199,199,199	0
57	MG	YB	203	1/1	0.89	0.07	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	XA	1651	1/1	0.89	0.10	43,43,43,43	0
57	MG	RA	3293	1/1	0.89	0.07	45,45,45,45	0
57	MG	RA	3205	1/1	0.89	0.15	61,61,61,61	0
57	MG	YA	3327	1/1	0.89	0.11	59,59,59,59	0
57	MG	YA	3173	1/1	0.89	0.17	54,54,54,54	0
57	MG	RA	3140	1/1	0.89	0.18	87,87,87,87	0
57	MG	XA	1624	1/1	0.90	0.07	70,70,70,70	0
57	MG	QA	1654	1/1	0.90	0.21	41,41,41,41	0
57	MG	YA	3179	1/1	0.90	0.13	46,46,46,46	0
57	MG	XA	1626	1/1	0.90	0.07	55,55,55,55	0
57	MG	QA	1623	1/1	0.90	0.08	87,87,87,87	0
57	MG	YA	3222	1/1	0.90	0.16	64,64,64,64	0
57	MG	XA	1633	1/1	0.90	0.26	46,46,46,46	0
57	MG	RA	3216	1/1	0.90	0.05	46,46,46,46	0
57	MG	YA	3009	1/1	0.90	0.10	47,47,47,47	0
57	MG	YA	3245	1/1	0.90	0.09	13,13,13,13	0
57	MG	YA	3010	1/1	0.90	0.20	11,11,11,11	0
57	MG	YA	3188	1/1	0.90	0.13	47,47,47,47	0
57	MG	YA	3022	1/1	0.90	0.30	11,11,11,11	0
57	MG	YA	3067	1/1	0.90	0.16	44,44,44,44	0
57	MG	YA	3192	1/1	0.90	0.14	55,55,55,55	0
57	MG	RA	3141	1/1	0.90	0.16	77,77,77,77	0
57	MG	QA	1624	1/1	0.90	0.08	84,84,84,84	0
57	MG	RA	3132	1/1	0.90	0.07	55,55,55,55	0
57	MG	XA	1648	1/1	0.90	0.14	61,61,61,61	0
57	MG	YA	3114	1/1	0.90	0.12	50,50,50,50	0
57	MG	RA	3271	1/1	0.90	0.15	56,56,56,56	0
57	MG	YA	3118	1/1	0.90	0.06	33,33,33,33	0
57	MG	RA	3189	1/1	0.90	0.11	70,70,70,70	0
57	MG	YA	3283	1/1	0.90	0.24	71,71,71,71	0
57	MG	RA	3134	1/1	0.90	0.16	62,62,62,62	0
57	MG	YA	3098	1/1	0.91	0.10	45,45,45,45	0
57	MG	XA	1631	1/1	0.91	0.12	44,44,44,44	0
57	MG	RA	3085	1/1	0.91	0.22	32,32,32,32	0
57	MG	RA	3319	1/1	0.91	0.11	27,27,27,27	0
57	MG	RA	3225	1/1	0.91	0.12	15,15,15,15	0
57	MG	YA	3116	1/1	0.91	0.13	30,30,30,30	0
57	MG	RA	3197	1/1	0.91	0.15	44,44,44,44	0
57	MG	YA	3119	1/1	0.91	0.14	60,60,60,60	0
57	MG	YA	3333	1/1	0.91	0.40	107,107,107,107	0
57	MG	RA	3329	1/1	0.91	0.15	34,34,34,34	0
57	MG	RA	3331	1/1	0.91	0.14	41,41,41,41	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	RA	3161	1/1	0.91	0.17	62,62,62,62	0
57	MG	RA	3088	1/1	0.91	0.17	28,28,28,28	0
57	MG	RA	3109	1/1	0.91	0.18	40,40,40,40	0
57	MG	QA	1629	1/1	0.91	0.28	71,71,71,71	0
57	MG	YA	3197	1/1	0.91	0.09	53,53,53,53	0
57	MG	YA	3199	1/1	0.91	0.10	35,35,35,35	0
57	MG	YA	3200	1/1	0.91	0.09	41,41,41,41	0
57	MG	RA	3292	1/1	0.91	0.08	80,80,80,80	0
57	MG	XA	1657	1/1	0.91	0.15	91,91,91,91	0
57	MG	XX	101	1/1	0.91	0.08	47,47,47,47	0
57	MG	QA	1613	1/1	0.91	0.06	56,56,56,56	0
57	MG	YA	3207	1/1	0.91	0.09	76,76,76,76	0
57	MG	YA	3208	1/1	0.91	0.09	60,60,60,60	0
57	MG	RA	3254	1/1	0.91	0.17	72,72,72,72	0
57	MG	Y3	101	1/1	0.91	0.17	66,66,66,66	0
57	MG	RA	3182	1/1	0.91	0.20	70,70,70,70	0
57	MG	RA	3300	1/1	0.91	0.09	57,57,57,57	0
57	MG	RA	3125	1/1	0.91	0.20	42,42,42,42	0
57	MG	RA	3305	1/1	0.91	0.06	52,52,52,52	0
57	MG	QA	1632	1/1	0.91	0.06	71,71,71,71	0
57	MG	RA	3309	1/1	0.91	0.14	47,47,47,47	0
57	MG	QA	1628	1/1	0.91	0.10	62,62,62,62	0
57	MG	YA	3080	1/1	0.91	0.15	51,51,51,51	0
57	MG	RA	3192	1/1	0.91	0.21	100,100,100,100	0
57	MG	YA	3217	1/1	0.92	0.06	63,63,63,63	0
57	MG	RA	3214	1/1	0.92	0.16	51,51,51,51	0
57	MG	YA	3303	1/1	0.92	0.13	51,51,51,51	0
57	MG	RA	3059	1/1	0.92	0.23	35,35,35,35	0
57	MG	YA	3308	1/1	0.92	0.11	41,41,41,41	0
57	MG	YA	3314	1/1	0.92	0.21	48,48,48,48	0
57	MG	YA	3092	1/1	0.92	0.15	86,86,86,86	0
57	MG	RA	3144	1/1	0.92	0.14	36,36,36,36	0
57	MG	YA	3176	1/1	0.92	0.14	53,53,53,53	0
57	MG	YA	3227	1/1	0.92	0.17	66,66,66,66	0
57	MG	YA	3228	1/1	0.92	0.18	72,72,72,72	0
57	MG	XA	1638	1/1	0.92	0.10	54,54,54,54	0
57	MG	YA	3233	1/1	0.92	0.07	47,47,47,47	0
57	MG	YA	3242	1/1	0.92	0.14	35,35,35,35	0
57	MG	RA	3318	1/1	0.92	0.23	50,50,50,50	0
57	MG	YA	3329	1/1	0.92	0.19	46,46,46,46	0
57	MG	YA	3112	1/1	0.92	0.12	40,40,40,40	0
57	MG	RA	3066	1/1	0.92	0.20	21,21,21,21	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	MG	RA	3320	1/1	0.92	0.09	36,36,36,36	0
57	MG	YA	3253	1/1	0.92	0.29	87,87,87,87	0
57	MG	QA	1627	1/1	0.92	0.06	62,62,62,62	0
57	MG	YA	3337	1/1	0.92	0.30	66,66,66,66	0
57	MG	RA	3278	1/1	0.92	0.22	63,63,63,63	0
57	MG	QA	1610	1/1	0.92	0.07	51,51,51,51	0
57	MG	RA	3158	1/1	0.92	0.15	26,26,26,26	0
57	MG	RA	3236	1/1	0.92	0.17	30,30,30,30	0
57	MG	RB	201	1/1	0.92	0.06	93,93,93,93	0
57	MG	RA	3160	1/1	0.92	0.09	48,48,48,48	0
57	MG	YA	3267	1/1	0.92	0.11	52,52,52,52	0
57	MG	YA	3346	1/1	0.92	0.15	50,50,50,50	0
57	MG	YA	3347	1/1	0.92	0.14	61,61,61,61	0
57	MG	YA	3129	1/1	0.92	0.14	86,86,86,86	0
57	MG	RA	3033	1/1	0.92	0.19	11,11,11,11	0
57	MG	RA	3107	1/1	0.92	0.18	78,78,78,78	0
57	MG	QA	1637	1/1	0.92	0.10	48,48,48,48	0
57	MG	YA	3357	1/1	0.92	0.10	27,27,27,27	0
57	MG	RA	3168	1/1	0.92	0.22	40,40,40,40	0
57	MG	RA	3298	1/1	0.92	0.15	61,61,61,61	0
57	MG	RA	3114	1/1	0.92	0.21	40,40,40,40	0
57	MG	RA	3257	1/1	0.92	0.07	21,21,21,21	0
57	MG	YA	3154	1/1	0.92	0.07	37,37,37,37	0
57	MG	RA	3301	1/1	0.92	0.18	41,41,41,41	0
57	MG	YA	3293	1/1	0.92	0.11	54,54,54,54	0
57	MG	RA	3258	1/1	0.92	0.12	47,47,47,47	0
57	MG	RA	3058	1/1	0.92	0.24	16,16,16,16	0
57	MG	YE	302	1/1	0.92	0.13	24,24,24,24	0
57	MG	YA	3037	1/1	0.92	0.22	9,9,9,9	0
57	MG	YP	202	1/1	0.92	0.13	25,25,25,25	0
57	MG	YA	3042	1/1	0.92	0.17	32,32,32,32	0
57	MG	RA	3176	1/1	0.92	0.13	29,29,29,29	0
57	MG	RA	3268	1/1	0.92	0.14	47,47,47,47	0
57	MG	QA	1653	1/1	0.93	0.05	65,65,65,65	0
57	MG	YA	3109	1/1	0.93	0.09	31,31,31,31	0
57	MG	YA	3177	1/1	0.93	0.13	47,47,47,47	0
57	MG	YA	3234	1/1	0.93	0.13	32,32,32,32	0
57	MG	RA	3256	1/1	0.93	0.18	30,30,30,30	0
57	MG	XA	1611	1/1	0.93	0.18	28,28,28,28	0
57	MG	RA	3316	1/1	0.93	0.06	31,31,31,31	0
57	MG	XA	1655	1/1	0.93	0.12	39,39,39,39	0
57	MG	QA	1622	1/1	0.93	0.09	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	XA	1658	1/1	0.93	0.15	83,83,83,83	0
57	MG	XV	102	1/1	0.93	0.09	29,29,29,29	0
57	MG	XA	1616	1/1	0.93	0.15	18,18,18,18	0
57	MG	XA	1618	1/1	0.93	0.18	57,57,57,57	0
57	MG	YA	3262	1/1	0.93	0.17	38,38,38,38	0
57	MG	RA	3157	1/1	0.93	0.13	25,25,25,25	0
57	MG	YA	3125	1/1	0.93	0.28	91,91,91,91	0
57	MG	RA	3202	1/1	0.93	0.15	48,48,48,48	0
57	MG	YA	3133	1/1	0.93	0.13	46,46,46,46	0
57	MG	YA	3196	1/1	0.93	0.05	73,73,73,73	0
57	MG	RA	3321	1/1	0.93	0.07	34,34,34,34	0
57	MG	YA	3278	1/1	0.93	0.09	20,20,20,20	0
57	MG	RA	3062	1/1	0.93	0.05	53,53,53,53	0
57	MG	YA	3006	1/1	0.93	0.17	24,24,24,24	0
57	MG	RA	3229	1/1	0.93	0.07	18,18,18,18	0
57	MG	YA	3144	1/1	0.93	0.07	32,32,32,32	0
57	MG	XA	1628	1/1	0.93	0.09	46,46,46,46	0
57	MG	RA	3185	1/1	0.93	0.07	61,61,61,61	0
57	MG	YA	3206	1/1	0.93	0.09	53,53,53,53	0
57	MG	YA	3353	1/1	0.93	0.48	74,74,74,74	0
57	MG	YA	3029	1/1	0.93	0.07	35,35,35,35	0
57	MG	RA	3237	1/1	0.93	0.10	23,23,23,23	0
57	MG	YA	3156	1/1	0.93	0.17	45,45,45,45	0
57	MG	RA	3243	1/1	0.93	0.15	76,76,76,76	0
57	MG	YA	3158	1/1	0.93	0.13	37,37,37,37	0
57	MG	YA	3159	1/1	0.93	0.10	51,51,51,51	0
57	MG	YA	3062	1/1	0.93	0.20	78,78,78,78	0
57	MG	R7	101	1/1	0.93	0.10	26,26,26,26	0
57	MG	QA	1615	1/1	0.93	0.07	52,52,52,52	0
57	MG	QA	1647	1/1	0.93	0.10	109,109,109,109	0
57	MG	XA	1645	1/1	0.93	0.11	45,45,45,45	0
57	MG	QA	1648	1/1	0.93	0.22	49,49,49,49	0
57	MG	RA	3089	1/1	0.93	0.12	15,15,15,15	0
57	MG	YA	3103	1/1	0.93	0.24	39,39,39,39	0
57	MG	YA	3310	1/1	0.93	0.13	41,41,41,41	0
57	MG	YA	3313	1/1	0.93	0.09	37,37,37,37	0
57	MG	RA	3311	1/1	0.93	0.10	50,50,50,50	0
57	MG	YY	201	1/1	0.93	0.09	41,41,41,41	0
57	MG	RA	3074	1/1	0.94	0.14	37,37,37,37	0
57	MG	YA	3306	1/1	0.94	0.21	54,54,54,54	0
57	MG	RA	3151	1/1	0.94	0.12	26,26,26,26	0
57	MG	YA	3160	1/1	0.94	0.13	29,29,29,29	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	RA	3077	1/1	0.94	0.14	20,20,20,20	0
57	MG	XA	1646	1/1	0.94	0.04	43,43,43,43	0
57	MG	RA	3218	1/1	0.94	0.06	35,35,35,35	0
57	MG	YA	3084	1/1	0.94	0.17	17,17,17,17	0
57	MG	YA	3224	1/1	0.94	0.15	43,43,43,43	0
57	MG	QA	1626	1/1	0.94	0.06	98,98,98,98	0
57	MG	YA	3097	1/1	0.94	0.18	40,40,40,40	0
57	MG	YA	3229	1/1	0.94	0.14	46,46,46,46	0
57	MG	RF	301	1/1	0.94	0.18	77,77,77,77	0
57	MG	YA	3101	1/1	0.94	0.08	51,51,51,51	0
57	MG	YA	3172	1/1	0.94	0.20	49,49,49,49	0
57	MG	RA	3223	1/1	0.94	0.11	11,11,11,11	0
57	MG	YA	3174	1/1	0.94	0.11	25,25,25,25	0
57	MG	RA	3155	1/1	0.94	0.17	48,48,48,48	0
57	MG	QA	1605	1/1	0.94	0.17	34,34,34,34	0
57	MG	YA	3249	1/1	0.94	0.07	44,44,44,44	0
57	MG	RA	3272	1/1	0.94	0.10	31,31,31,31	0
57	MG	R5	101	1/1	0.94	0.14	58,58,58,58	0
57	MG	YA	3256	1/1	0.94	0.24	47,47,47,47	0
57	MG	RA	3093	1/1	0.94	0.11	25,25,25,25	0
57	MG	RA	3105	1/1	0.94	0.10	32,32,32,32	0
57	MG	RA	3022	1/1	0.94	0.28	28,28,28,28	0
57	MG	QA	1652	1/1	0.94	0.08	61,61,61,61	0
57	MG	RA	3042	1/1	0.94	0.09	17,17,17,17	0
57	MG	RA	3204	1/1	0.94	0.16	66,66,66,66	0
57	MG	RA	3115	1/1	0.94	0.08	22,22,22,22	0
57	MG	RA	3119	1/1	0.94	0.12	34,34,34,34	0
57	MG	RA	3146	1/1	0.94	0.09	63,63,63,63	0
57	MG	RA	3327	1/1	0.94	0.23	50,50,50,50	0
57	MG	YA	3270	1/1	0.94	0.14	58,58,58,58	0
57	MG	YA	3274	1/1	0.94	0.10	26,26,26,26	0
57	MG	YA	3352	1/1	0.94	0.21	74,74,74,74	0
57	MG	RA	3253	1/1	0.94	0.15	40,40,40,40	0
57	MG	YA	3131	1/1	0.94	0.12	21,21,21,21	0
57	MG	YA	3132	1/1	0.94	0.14	56,56,56,56	0
57	MG	XA	1634	1/1	0.94	0.14	45,45,45,45	0
57	MG	YA	3017	1/1	0.94	0.15	32,32,32,32	0
57	MG	XA	1635	1/1	0.94	0.05	23,23,23,23	0
57	MG	YA	3138	1/1	0.94	0.14	34,34,34,34	0
57	MG	RA	3178	1/1	0.94	0.07	28,28,28,28	0
57	MG	YA	3032	1/1	0.94	0.32	29,29,29,29	0
57	MG	YA	3033	1/1	0.94	0.12	30,30,30,30	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	RA	3297	1/1	0.94	0.27	50,50,50,50	0
57	MG	YA	3147	1/1	0.94	0.19	45,45,45,45	0
57	MG	YA	3148	1/1	0.94	0.18	50,50,50,50	0
57	MG	YA	3039	1/1	0.94	0.21	18,18,18,18	0
57	MG	YA	3040	1/1	0.94	0.17	24,24,24,24	0
57	MG	XA	1640	1/1	0.94	0.22	26,26,26,26	0
57	MG	YA	3049	1/1	0.94	0.14	47,47,47,47	0
57	MG	YA	3051	1/1	0.94	0.17	21,21,21,21	0
57	MG	YA	3215	1/1	0.94	0.15	15,15,15,15	0
57	MG	YA	3078	1/1	0.95	0.14	8,8,8,8	0
57	MG	YA	3079	1/1	0.95	0.08	44,44,44,44	0
57	MG	YA	3284	1/1	0.95	0.30	86,86,86,86	0
57	MG	YA	3285	1/1	0.95	0.18	50,50,50,50	0
57	MG	QA	1650	1/1	0.95	0.08	14,14,14,14	0
57	MG	YA	3183	1/1	0.95	0.07	45,45,45,45	0
57	MG	YA	3289	1/1	0.95	0.12	52,52,52,52	0
57	MG	RA	3110	1/1	0.95	0.11	21,21,21,21	0
57	MG	RA	3112	1/1	0.95	0.12	74,74,74,74	0
57	MG	YA	3087	1/1	0.95	0.14	41,41,41,41	0
57	MG	RA	3054	1/1	0.95	0.11	20,20,20,20	0
57	MG	RA	3008	1/1	0.95	0.14	11,11,11,11	0
57	MG	QA	1651	1/1	0.95	0.12	34,34,34,34	0
57	MG	QA	1612	1/1	0.95	0.13	46,46,46,46	0
57	MG	QA	1618	1/1	0.95	0.07	39,39,39,39	0
57	MG	YA	3194	1/1	0.95	0.22	22,22,22,22	0
57	MG	RA	3235	1/1	0.95	0.06	14,14,14,14	0
57	MG	RA	3302	1/1	0.95	0.07	23,23,23,23	0
57	MG	YA	3107	1/1	0.95	0.05	9,9,9,9	0
57	MG	QA	1609	1/1	0.95	0.07	62,62,62,62	0
57	MG	YA	3305	1/1	0.95	0.07	60,60,60,60	0
57	MG	RA	3174	1/1	0.95	0.08	38,38,38,38	0
57	MG	RA	3306	1/1	0.95	0.07	44,44,44,44	0
57	MG	RA	3126	1/1	0.95	0.09	54,54,54,54	0
57	MG	YA	3309	1/1	0.95	0.05	52,52,52,52	0
57	MG	RA	3128	1/1	0.95	0.10	20,20,20,20	0
57	MG	YA	3311	1/1	0.95	0.20	46,46,46,46	0
57	MG	YA	3312	1/1	0.95	0.06	22,22,22,22	0
57	MG	RA	3072	1/1	0.95	0.18	25,25,25,25	0
57	MG	R0	101	1/1	0.95	0.08	19,19,19,19	0
57	MG	QA	1620	1/1	0.95	0.10	41,41,41,41	0
57	MG	YA	3316	1/1	0.95	0.09	49,49,49,49	0
57	MG	RA	3313	1/1	0.95	0.08	46,46,46,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	RA	3188	1/1	0.95	0.13	50,50,50,50	0
57	MG	YA	3320	1/1	0.95	0.12	15,15,15,15	0
57	MG	RA	3081	1/1	0.95	0.16	49,49,49,49	0
57	MG	RA	3317	1/1	0.95	0.07	45,45,45,45	0
57	MG	RA	3027	1/1	0.95	0.11	16,16,16,16	0
57	MG	YA	3130	1/1	0.95	0.20	21,21,21,21	0
57	MG	QA	1625	1/1	0.95	0.20	27,27,27,27	0
57	MG	RA	3194	1/1	0.95	0.09	55,55,55,55	0
57	MG	RA	3195	1/1	0.95	0.10	35,35,35,35	0
57	MG	RA	3259	1/1	0.95	0.20	43,43,43,43	0
57	MG	RA	3323	1/1	0.95	0.15	30,30,30,30	0
57	MG	RA	3325	1/1	0.95	0.13	27,27,27,27	0
57	MG	RA	3260	1/1	0.95	0.18	35,35,35,35	0
57	MG	RA	3139	1/1	0.95	0.06	16,16,16,16	0
57	MG	RA	3262	1/1	0.95	0.12	58,58,58,58	0
57	MG	RA	3330	1/1	0.95	0.05	32,32,32,32	0
57	MG	RA	3266	1/1	0.95	0.15	22,22,22,22	0
57	MG	RA	3332	1/1	0.95	0.12	103,103,103,103	0
57	MG	YA	3149	1/1	0.95	0.18	85,85,85,85	0
57	MG	RA	3034	1/1	0.95	0.19	24,24,24,24	0
57	MG	YA	3239	1/1	0.95	0.10	32,32,32,32	0
57	MG	RA	3090	1/1	0.95	0.15	43,43,43,43	0
57	MG	RA	3142	1/1	0.95	0.09	62,62,62,62	0
57	MG	RA	3092	1/1	0.95	0.18	15,15,15,15	0
57	MG	RA	3145	1/1	0.95	0.08	34,34,34,34	0
57	MG	RA	3039	1/1	0.95	0.22	21,21,21,21	0
57	MG	RA	3148	1/1	0.95	0.20	74,74,74,74	0
57	MG	RR	201	1/1	0.95	0.13	21,21,21,21	0
57	MG	YA	3038	1/1	0.95	0.22	39,39,39,39	0
57	MG	RA	3276	1/1	0.95	0.05	35,35,35,35	0
57	MG	RA	3208	1/1	0.95	0.09	22,22,22,22	0
57	MG	RA	3099	1/1	0.95	0.11	59,59,59,59	0
57	MG	YA	3046	1/1	0.95	0.14	43,43,43,43	0
57	MG	RA	3102	1/1	0.95	0.07	33,33,33,33	0
57	MG	YA	3050	1/1	0.95	0.14	40,40,40,40	0
57	MG	RA	3040	1/1	0.95	0.13	27,27,27,27	0
57	MG	YA	3052	1/1	0.95	0.10	16,16,16,16	0
57	MG	YA	3061	1/1	0.95	0.25	31,31,31,31	0
57	MG	QA	1640	1/1	0.95	0.07	84,84,84,84	0
57	MG	YA	3065	1/1	0.95	0.19	32,32,32,32	0
57	MG	YA	3271	1/1	0.95	0.21	56,56,56,56	0
57	MG	YA	3273	1/1	0.95	0.05	32,32,32,32	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	MG	RA	3288	1/1	0.95	0.16	48,48,48,48	0
57	MG	YA	3276	1/1	0.95	0.26	89,89,89,89	0
57	MG	RA	3108	1/1	0.95	0.09	63,63,63,63	0
57	MG	YA	3074	1/1	0.95	0.16	12,12,12,12	0
57	MG	YA	3076	1/1	0.95	0.16	17,17,17,17	0
57	MG	YA	3201	1/1	0.96	0.07	46,46,46,46	0
57	MG	RA	3308	1/1	0.96	0.12	58,58,58,58	0
57	MG	YA	3019	1/1	0.96	0.16	16,16,16,16	0
57	MG	XA	1615	1/1	0.96	0.24	37,37,37,37	0
57	MG	RA	3265	1/1	0.96	0.21	44,44,44,44	0
57	MG	XA	1617	1/1	0.96	0.22	28,28,28,28	0
57	MG	RA	3180	1/1	0.96	0.10	63,63,63,63	0
57	MG	XA	1620	1/1	0.96	0.21	24,24,24,24	0
57	MG	YA	3137	1/1	0.96	0.07	38,38,38,38	0
57	MG	RA	3181	1/1	0.96	0.13	22,22,22,22	0
57	MG	RA	3050	1/1	0.96	0.14	29,29,29,29	0
57	MG	YA	3140	1/1	0.96	0.11	43,43,43,43	0
57	MG	RA	3183	1/1	0.96	0.19	75,75,75,75	0
57	MG	YA	3143	1/1	0.96	0.09	67,67,67,67	0
57	MG	RA	3094	1/1	0.96	0.17	13,13,13,13	0
57	MG	RA	3097	1/1	0.96	0.13	21,21,21,21	0
57	MG	YA	3048	1/1	0.96	0.16	13,13,13,13	0
57	MG	RA	3150	1/1	0.96	0.05	20,20,20,20	0
57	MG	RA	3071	1/1	0.96	0.14	27,27,27,27	0
57	MG	YA	3150	1/1	0.96	0.07	49,49,49,49	0
57	MG	RA	3231	1/1	0.96	0.20	40,40,40,40	0
57	MG	RA	3051	1/1	0.96	0.05	25,25,25,25	0
57	MG	YA	3053	1/1	0.96	0.13	12,12,12,12	0
57	MG	YA	3317	1/1	0.96	0.18	40,40,40,40	0
57	MG	RA	3030	1/1	0.96	0.16	42,42,42,42	0
57	MG	XA	1636	1/1	0.96	0.20	56,56,56,56	0
57	MG	RA	3280	1/1	0.96	0.34	57,57,57,57	0
57	MG	RA	3076	1/1	0.96	0.08	25,25,25,25	0
57	MG	RA	3324	1/1	0.96	0.11	8,8,8,8	0
57	MG	YA	3238	1/1	0.96	0.11	27,27,27,27	0
57	MG	XA	1641	1/1	0.96	0.04	77,77,77,77	0
57	MG	YA	3240	1/1	0.96	0.14	7,7,7,7	0
57	MG	RA	3239	1/1	0.96	0.11	30,30,30,30	0
57	MG	RA	3285	1/1	0.96	0.17	49,49,49,49	0
57	MG	YA	3330	1/1	0.96	0.09	28,28,28,28	0
57	MG	YA	3165	1/1	0.96	0.06	49,49,49,49	0
57	MG	RA	3002	1/1	0.96	0.33	294,294,294,294	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	YA	3248	1/1	0.96	0.13	11,11,11,11	0
57	MG	RA	3287	1/1	0.96	0.14	45,45,45,45	0
57	MG	RA	3244	1/1	0.96	0.19	52,52,52,52	0
57	MG	RA	3133	1/1	0.96	0.11	39,39,39,39	0
57	MG	YA	3085	1/1	0.96	0.08	23,23,23,23	0
57	MG	YA	3086	1/1	0.96	0.08	48,48,48,48	0
57	MG	YA	3258	1/1	0.96	0.07	16,16,16,16	0
57	MG	RA	3247	1/1	0.96	0.09	46,46,46,46	0
57	MG	RA	3159	1/1	0.96	0.10	30,30,30,30	0
57	MG	YA	3096	1/1	0.96	0.05	27,27,27,27	0
57	MG	QA	1608	1/1	0.96	0.09	49,49,49,49	0
57	MG	RA	3135	1/1	0.96	0.11	76,76,76,76	0
57	MG	RA	3137	1/1	0.96	0.07	11,11,11,11	0
57	MG	QA	1604	1/1	0.96	0.07	51,51,51,51	0
57	MG	RA	3166	1/1	0.96	0.04	53,53,53,53	0
57	MG	RA	3087	1/1	0.96	0.25	30,30,30,30	0
57	MG	YA	3269	1/1	0.96	0.08	32,32,32,32	0
57	MG	QA	1601	1/1	0.96	0.08	36,36,36,36	0
57	MG	RA	3064	1/1	0.96	0.26	16,16,16,16	0
57	MG	XA	1601	1/1	0.96	0.17	28,28,28,28	0
57	MG	YA	3185	1/1	0.96	0.17	54,54,54,54	0
57	MG	RA	3116	1/1	0.96	0.06	49,49,49,49	0
57	MG	YA	3277	1/1	0.96	0.13	34,34,34,34	0
57	MG	QA	1634	1/1	0.96	0.10	50,50,50,50	0
57	MG	XA	1605	1/1	0.96	0.05	51,51,51,51	0
57	MG	YA	3280	1/1	0.96	0.23	86,86,86,86	0
57	MG	XA	1607	1/1	0.96	0.17	22,22,22,22	0
57	MG	YA	3005	1/1	0.96	0.07	25,25,25,25	0
57	MG	XA	1610	1/1	0.96	0.06	40,40,40,40	0
57	MG	RA	3177	1/1	0.96	0.05	35,35,35,35	0
57	MG	YA	3122	1/1	0.96	0.14	22,22,22,22	0
57	MG	RA	3069	1/1	0.96	0.06	46,46,46,46	0
57	MG	YA	3014	1/1	0.96	0.15	49,49,49,49	0
57	MG	YA	3198	1/1	0.96	0.18	39,39,39,39	0
57	MG	YA	3015	1/1	0.96	0.06	14,14,14,14	0
57	MG	YA	3128	1/1	0.96	0.14	41,41,41,41	0
57	MG	Y5	101	1/1	0.97	0.05	23,23,23,23	0
57	MG	YA	3141	1/1	0.97	0.07	19,19,19,19	0
57	MG	RA	3083	1/1	0.97	0.10	22,22,22,22	0
57	MG	RA	3127	1/1	0.97	0.14	1,1,1,1	0
57	MG	RA	3044	1/1	0.97	0.11	32,32,32,32	0
57	MG	YA	3145	1/1	0.97	0.14	67,67,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	RA	3047	1/1	0.97	0.15	20,20,20,20	0
57	MG	YA	3007	1/1	0.97	0.06	22,22,22,22	0
57	MG	QA	1631	1/1	0.97	0.04	39,39,39,39	0
57	MG	RA	3013	1/1	0.97	0.08	17,17,17,17	0
57	MG	QA	1602	1/1	0.97	0.23	33,33,33,33	0
57	MG	RA	3091	1/1	0.97	0.13	30,30,30,30	0
57	MG	RA	3187	1/1	0.97	0.04	55,55,55,55	0
57	MG	YA	3153	1/1	0.97	0.05	2,2,2,2	0
57	MG	RA	3019	1/1	0.97	0.11	26,26,26,26	0
57	MG	QA	1616	1/1	0.97	0.10	40,40,40,40	0
57	MG	YA	3023	1/1	0.97	0.18	20,20,20,20	0
57	MG	YA	3024	1/1	0.97	0.05	34,34,34,34	0
57	MG	YA	3025	1/1	0.97	0.09	22,22,22,22	0
57	MG	RA	3026	1/1	0.97	0.15	13,13,13,13	0
57	MG	YA	3031	1/1	0.97	0.10	13,13,13,13	0
57	MG	RA	3263	1/1	0.97	0.07	53,53,53,53	0
57	MG	RA	3264	1/1	0.97	0.17	31,31,31,31	0
57	MG	RA	3095	1/1	0.97	0.08	15,15,15,15	0
57	MG	RA	3096	1/1	0.97	0.12	14,14,14,14	0
57	MG	RA	3060	1/1	0.97	0.15	18,18,18,18	0
57	MG	RA	3004	1/1	0.97	0.16	21,21,21,21	0
57	MG	RA	3269	1/1	0.97	0.05	29,29,29,29	0
57	MG	YA	3043	1/1	0.97	0.12	11,11,11,11	0
57	MG	RA	3100	1/1	0.97	0.07	14,14,14,14	0
57	MG	YA	3047	1/1	0.97	0.07	7,7,7,7	0
57	MG	RA	3198	1/1	0.97	0.10	30,30,30,30	0
57	MG	RA	3199	1/1	0.97	0.21	41,41,41,41	0
57	MG	RA	3101	1/1	0.97	0.05	53,53,53,53	0
57	MG	XA	1606	1/1	0.97	0.04	30,30,30,30	0
57	MG	RA	3028	1/1	0.97	0.08	17,17,17,17	0
57	MG	YA	3297	1/1	0.97	0.20	36,36,36,36	0
57	MG	RA	3275	1/1	0.97	0.10	51,51,51,51	0
57	MG	YA	3055	1/1	0.97	0.16	30,30,30,30	0
57	MG	YA	3060	1/1	0.97	0.05	26,26,26,26	0
57	MG	RA	3104	1/1	0.97	0.07	17,17,17,17	0
57	MG	XA	1612	1/1	0.97	0.21	46,46,46,46	0
57	MG	YA	3063	1/1	0.97	0.09	26,26,26,26	0
57	MG	RA	3005	1/1	0.97	0.13	16,16,16,16	0
57	MG	RA	3106	1/1	0.97	0.06	23,23,23,23	0
57	MG	YA	3068	1/1	0.97	0.14	17,17,17,17	0
57	MG	RA	3031	1/1	0.97	0.13	22,22,22,22	0
57	MG	YA	3189	1/1	0.97	0.17	32,32,32,32	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	RA	3006	1/1	0.97	0.17	11,11,11,11	0
57	MG	RA	3152	1/1	0.97	0.09	48,48,48,48	0
57	MG	RA	3284	1/1	0.97	0.07	34,34,34,34	0
57	MG	QA	1617	1/1	0.97	0.08	43,43,43,43	0
57	MG	RA	3037	1/1	0.97	0.09	22,22,22,22	0
57	MG	YA	3195	1/1	0.97	0.10	44,44,44,44	0
57	MG	YA	3081	1/1	0.97	0.14	11,11,11,11	0
57	MG	XA	1623	1/1	0.97	0.22	61,61,61,61	0
57	MG	RA	3212	1/1	0.97	0.14	27,27,27,27	0
57	MG	RA	3111	1/1	0.97	0.11	35,35,35,35	0
57	MG	RA	3289	1/1	0.97	0.05	53,53,53,53	0
57	MG	YA	3321	1/1	0.97	0.06	48,48,48,48	0
57	MG	RA	3073	1/1	0.97	0.08	40,40,40,40	0
57	MG	YA	3090	1/1	0.97	0.10	17,17,17,17	0
57	MG	RA	3113	1/1	0.97	0.06	32,32,32,32	0
57	MG	YA	3093	1/1	0.97	0.12	11,11,11,11	0
57	MG	YA	3095	1/1	0.97	0.04	41,41,41,41	0
57	MG	RA	3217	1/1	0.97	0.08	48,48,48,48	0
57	MG	XA	1632	1/1	0.97	0.12	20,20,20,20	0
57	MG	QA	1607	1/1	0.97	0.14	26,26,26,26	0
57	MG	YA	3209	1/1	0.97	0.08	43,43,43,43	0
57	MG	RA	3295	1/1	0.97	0.17	36,36,36,36	0
57	MG	RA	3219	1/1	0.97	0.12	44,44,44,44	0
57	MG	YA	3334	1/1	0.97	0.05	17,17,17,17	0
57	MG	QA	1644	1/1	0.97	0.09	40,40,40,40	0
57	MG	RA	3221	1/1	0.97	0.19	21,21,21,21	0
57	MG	RA	3041	1/1	0.97	0.10	20,20,20,20	0
57	MG	RA	3162	1/1	0.97	0.04	34,34,34,34	0
57	MG	YA	3111	1/1	0.97	0.14	12,12,12,12	0
57	MG	RA	3117	1/1	0.97	0.07	49,49,49,49	0
57	MG	XA	1642	1/1	0.97	0.21	41,41,41,41	0
57	MG	YA	3342	1/1	0.97	0.06	53,53,53,53	0
57	MG	RA	3078	1/1	0.97	0.08	42,42,42,42	0
57	MG	RA	3228	1/1	0.97	0.05	21,21,21,21	0
57	MG	RA	3079	1/1	0.97	0.07	6,6,6,6	0
57	MG	RA	3167	1/1	0.97	0.05	36,36,36,36	0
57	MG	RA	3232	1/1	0.97	0.13	30,30,30,30	0
57	MG	YA	3226	1/1	0.97	0.15	46,46,46,46	0
57	MG	RA	3233	1/1	0.97	0.12	34,34,34,34	0
57	MG	RA	3234	1/1	0.97	0.22	23,23,23,23	0
57	MG	YA	3351	1/1	0.97	0.24	76,76,76,76	0
57	MG	RA	3121	1/1	0.97	0.14	41,41,41,41	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	MG	YA	3230	1/1	0.97	0.14	14,14,14,14	0
57	MG	RA	3169	1/1	0.97	0.05	35,35,35,35	0
57	MG	YA	3355	1/1	0.97	0.06	27,27,27,27	0
57	MG	RA	3122	1/1	0.97	0.13	33,33,33,33	0
57	MG	YA	3127	1/1	0.97	0.16	18,18,18,18	0
57	MG	YA	3235	1/1	0.97	0.05	16,16,16,16	0
57	MG	YA	3236	1/1	0.97	0.13	13,13,13,13	0
57	MG	XA	1653	1/1	0.97	0.09	56,56,56,56	0
57	MG	RA	3123	1/1	0.97	0.15	54,54,54,54	0
57	MG	RA	3314	1/1	0.97	0.04	58,58,58,58	0
57	MG	YA	3241	1/1	0.97	0.16	13,13,13,13	0
57	MG	XA	1656	1/1	0.97	0.06	74,74,74,74	0
57	MG	RA	3241	1/1	0.97	0.07	26,26,26,26	0
57	MG	RA	3172	1/1	0.97	0.05	26,26,26,26	0
57	MG	YA	3134	1/1	0.97	0.03	53,53,53,53	0
57	MG	RA	3173	1/1	0.97	0.04	30,30,30,30	0
57	MG	YQ	201	1/1	0.97	0.13	25,25,25,25	0
57	MG	RA	3245	1/1	0.97	0.11	23,23,23,23	0
57	MG	R8	101	1/1	0.97	0.23	49,49,49,49	0
57	MG	RA	3175	1/1	0.97	0.07	35,35,35,35	0
57	MG	RA	3082	1/1	0.97	0.09	9,9,9,9	0
59	ZN	QN	100	1/1	0.97	0.05	136,136,136,136	0
57	MG	XA	1602	1/1	0.98	0.24	43,43,43,43	0
57	MG	YA	3088	1/1	0.98	0.10	44,44,44,44	0
57	MG	YA	3089	1/1	0.98	0.04	9,9,9,9	0
57	MG	QA	1643	1/1	0.98	0.08	38,38,38,38	0
57	MG	YA	3091	1/1	0.98	0.05	9,9,9,9	0
57	MG	RA	3052	1/1	0.98	0.09	11,11,11,11	0
57	MG	QV	101	1/1	0.98	0.08	54,54,54,54	0
57	MG	RA	3252	1/1	0.98	0.05	66,66,66,66	0
57	MG	RA	3086	1/1	0.98	0.09	31,31,31,31	0
57	MG	XA	1608	1/1	0.98	0.07	49,49,49,49	0
57	MG	XA	1609	1/1	0.98	0.21	42,42,42,42	0
57	MG	YA	3099	1/1	0.98	0.11	33,33,33,33	0
57	MG	YA	3100	1/1	0.98	0.06	12,12,12,12	0
57	MG	YA	3001	1/1	0.98	0.12	52,52,52,52	0
57	MG	YA	3002	1/1	0.98	0.09	18,18,18,18	0
57	MG	RA	3029	1/1	0.98	0.12	16,16,16,16	0
57	MG	RA	3255	1/1	0.98	0.14	52,52,52,52	0
57	MG	RA	3143	1/1	0.98	0.09	15,15,15,15	0
57	MG	YA	3008	1/1	0.98	0.11	35,35,35,35	0
57	MG	YA	3110	1/1	0.98	0.12	11,11,11,11	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	QA	1649	1/1	0.98	0.05	60,60,60,60	0
57	MG	RA	3304	1/1	0.98	0.18	75,75,75,75	0
57	MG	YA	3113	1/1	0.98	0.07	36,36,36,36	0
57	MG	QA	1614	1/1	0.98	0.03	76,76,76,76	0
57	MG	RA	3032	1/1	0.98	0.16	7,7,7,7	0
57	MG	YA	3304	1/1	0.98	0.32	40,40,40,40	0
57	MG	YA	3016	1/1	0.98	0.10	10,10,10,10	0
57	MG	RA	3179	1/1	0.98	0.13	74,74,74,74	0
57	MG	YA	3018	1/1	0.98	0.10	11,11,11,11	0
57	MG	RA	3147	1/1	0.98	0.13	36,36,36,36	0
57	MG	YA	3021	1/1	0.98	0.13	28,28,28,28	0
57	MG	XA	1619	1/1	0.98	0.11	33,33,33,33	0
57	MG	RA	3118	1/1	0.98	0.11	26,26,26,26	0
57	MG	XA	1621	1/1	0.98	0.18	12,12,12,12	0
57	MG	QA	1636	1/1	0.98	0.07	68,68,68,68	0
57	MG	YA	3026	1/1	0.98	0.09	28,28,28,28	0
57	MG	YA	3027	1/1	0.98	0.09	19,19,19,19	0
57	MG	RA	3015	1/1	0.98	0.04	2,2,2,2	0
57	MG	YA	3030	1/1	0.98	0.14	13,13,13,13	0
57	MG	RA	3222	1/1	0.98	0.13	11,11,11,11	0
57	MG	YA	3219	1/1	0.98	0.11	38,38,38,38	0
57	MG	RA	3184	1/1	0.98	0.07	21,21,21,21	0
57	MG	RA	3065	1/1	0.98	0.10	27,27,27,27	0
57	MG	YA	3034	1/1	0.98	0.21	15,15,15,15	0
57	MG	YA	3036	1/1	0.98	0.04	15,15,15,15	0
57	MG	RA	3036	1/1	0.98	0.06	15,15,15,15	0
57	MG	YA	3325	1/1	0.98	0.10	20,20,20,20	0
57	MG	RA	3067	1/1	0.98	0.10	18,18,18,18	0
57	MG	XA	1629	1/1	0.98	0.09	58,58,58,58	0
57	MG	XA	1630	1/1	0.98	0.06	70,70,70,70	0
57	MG	YA	3041	1/1	0.98	0.21	32,32,32,32	0
57	MG	RA	3227	1/1	0.98	0.10	21,21,21,21	0
57	MG	RA	3016	1/1	0.98	0.06	4,4,4,4	0
57	MG	YA	3232	1/1	0.98	0.10	25,25,25,25	0
57	MG	RA	3017	1/1	0.98	0.05	22,22,22,22	0
57	MG	RA	3230	1/1	0.98	0.15	23,23,23,23	0
57	MG	RA	3156	1/1	0.98	0.08	36,36,36,36	0
57	MG	RA	3191	1/1	0.98	0.05	52,52,52,52	0
57	MG	YA	3237	1/1	0.98	0.21	18,18,18,18	0
57	MG	XA	1637	1/1	0.98	0.03	45,45,45,45	0
57	MG	RA	3007	1/1	0.98	0.10	8,8,8,8	0
57	MG	RA	3193	1/1	0.98	0.07	46,46,46,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	MG	RA	3020	1/1	0.98	0.10	21,21,21,21	0
57	MG	RA	3279	1/1	0.98	0.21	33,33,33,33	0
57	MG	YA	3057	1/1	0.98	0.12	11,11,11,11	0
57	MG	YA	3058	1/1	0.98	0.13	19,19,19,19	0
57	MG	YA	3246	1/1	0.98	0.09	6,6,6,6	0
57	MG	YA	3059	1/1	0.98	0.06	19,19,19,19	0
57	MG	QA	1633	1/1	0.98	0.04	28,28,28,28	0
57	MG	RA	3328	1/1	0.98	0.12	36,36,36,36	0
57	MG	YA	3250	1/1	0.98	0.18	20,20,20,20	0
57	MG	YA	3251	1/1	0.98	0.19	68,68,68,68	0
57	MG	RA	3043	1/1	0.98	0.09	21,21,21,21	0
57	MG	RA	3282	1/1	0.98	0.12	22,22,22,22	0
57	MG	YA	3255	1/1	0.98	0.07	28,28,28,28	0
57	MG	YA	3064	1/1	0.98	0.09	11,11,11,11	0
57	MG	RA	3238	1/1	0.98	0.11	37,37,37,37	0
57	MG	RA	3103	1/1	0.98	0.05	20,20,20,20	0
57	MG	YA	3259	1/1	0.98	0.09	25,25,25,25	0
57	MG	YA	3163	1/1	0.98	0.13	18,18,18,18	0
57	MG	RA	3240	1/1	0.98	0.22	26,26,26,26	0
57	MG	RA	3075	1/1	0.98	0.03	44,44,44,44	0
57	MG	YA	3072	1/1	0.98	0.08	36,36,36,36	0
57	MG	YA	3073	1/1	0.98	0.04	16,16,16,16	0
57	MG	RA	3242	1/1	0.98	0.04	21,21,21,21	0
57	MG	RA	3023	1/1	0.98	0.06	40,40,40,40	0
57	MG	YA	3077	1/1	0.98	0.10	19,19,19,19	0
57	MG	RA	3045	1/1	0.98	0.11	16,16,16,16	0
57	MG	RA	3025	1/1	0.98	0.05	27,27,27,27	0
57	MG	RE	301	1/1	0.98	0.07	7,7,7,7	0
57	MG	RA	3048	1/1	0.98	0.08	17,17,17,17	0
57	MG	RA	3136	1/1	0.98	0.06	9,9,9,9	0
57	MG	QA	1603	1/1	0.98	0.11	72,72,72,72	0
57	MG	YA	3275	1/1	0.98	0.13	34,34,34,34	0
57	MG	RA	3294	1/1	0.98	0.07	46,46,46,46	0
58	SF4	QD	301	8/8	0.98	0.05	71,100,181,225	0
58	SF4	XD	301	8/8	0.98	0.07	70,85,155,236	0
57	MG	XV	101	1/1	0.98	0.07	64,64,64,64	0
59	ZN	XN	101	1/1	0.98	0.04	149,149,149,149	0
57	MG	YA	3056	1/1	0.99	0.06	13,13,13,13	0
57	MG	YA	3003	1/1	0.99	0.05	27,27,27,27	0
57	MG	YA	3028	1/1	0.99	0.12	1,1,1,1	0
57	MG	YA	3094	1/1	0.99	0.05	30,30,30,30	0
57	MG	YA	3004	1/1	0.99	0.07	41,41,41,41	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	RA	3046	1/1	0.99	0.05	30,30,30,30	0
57	MG	RA	3021	1/1	0.99	0.07	15,15,15,15	0
57	MG	RA	3084	1/1	0.99	0.04	11,11,11,11	0
57	MG	RA	3098	1/1	0.99	0.04	3,3,3,3	0
57	MG	RA	3061	1/1	0.99	0.15	15,15,15,15	0
57	MG	YA	3035	1/1	0.99	0.07	18,18,18,18	0
57	MG	YA	3102	1/1	0.99	0.11	21,21,21,21	0
57	MG	RA	3024	1/1	0.99	0.12	11,11,11,11	0
57	MG	YA	3104	1/1	0.99	0.14	11,11,11,11	0
57	MG	YA	3011	1/1	0.99	0.10	1,1,1,1	0
57	MG	YA	3012	1/1	0.99	0.05	12,12,12,12	0
57	MG	YA	3013	1/1	0.99	0.04	11,11,11,11	0
57	MG	RA	3063	1/1	0.99	0.23	16,16,16,16	0
57	MG	YA	3225	1/1	0.99	0.03	24,24,24,24	0
57	MG	RA	3049	1/1	0.99	0.04	7,7,7,7	0
57	MG	YA	3075	1/1	0.99	0.03	17,17,17,17	0
57	MG	YA	3356	1/1	0.99	0.09	38,38,38,38	0
57	MG	RA	3055	1/1	0.99	0.06	14,14,14,14	0
57	MG	RA	3056	1/1	0.99	0.06	12,12,12,12	0
57	MG	YA	3272	1/1	0.99	0.06	67,67,67,67	0
57	MG	YA	3044	1/1	0.99	0.07	17,17,17,17	0
57	MG	YA	3045	1/1	0.99	0.07	11,11,11,11	0
57	MG	RA	3206	1/1	0.99	0.02	68,68,68,68	0
57	MG	YA	3117	1/1	0.99	0.05	13,13,13,13	0
57	MG	YA	3155	1/1	0.99	0.07	9,9,9,9	0
57	MG	RA	3207	1/1	0.99	0.02	51,51,51,51	0
57	MG	YA	3082	1/1	0.99	0.05	12,12,12,12	0
57	MG	YA	3020	1/1	0.99	0.04	3,3,3,3	0
57	MG	RA	3057	1/1	0.99	0.08	13,13,13,13	0
57	MG	RA	3068	1/1	0.99	0.11	21,21,21,21	0
57	MG	RA	3080	1/1	0.99	0.03	16,16,16,16	0
57	MG	RA	3164	1/1	0.99	0.06	26,26,26,26	0
57	MG	QA	1606	1/1	0.99	0.18	12,12,12,12	0
57	MG	YA	3286	1/1	0.99	0.13	33,33,33,33	0
57	MG	YA	3243	1/1	0.99	0.14	13,13,13,13	0
57	MG	YA	3126	1/1	0.99	0.03	31,31,31,31	0
57	MG	YA	3054	1/1	0.99	0.07	11,11,11,11	0
57	MG	RA	3213	1/1	0.99	0.04	45,45,45,45	0
57	MG	YA	3167	1/1	0.99	0.09	35,35,35,35	0
57	MG	RA	3038	1/1	1.00	0.04	11,11,11,11	0
57	MG	YA	3069	1/1	1.00	0.02	15,15,15,15	0
57	MG	RA	3018	1/1	1.00	0.07	15,15,15,15	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	YA	3254	1/1	1.00	0.04	12,12,12,12	0
57	MG	YA	3071	1/1	1.00	0.06	22,22,22,22	0
57	MG	YA	3108	1/1	1.00	0.04	19,19,19,19	0
57	MG	YA	3066	1/1	1.00	0.03	4,4,4,4	0
57	MG	RA	3035	1/1	1.00	0.03	5,5,5,5	0

5.5 Other polymers [i](#)

There are no such residues in this entry.