



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 11:54 AM UTC

PDB ID : 4LEL / pdb_00004lel
Title : Crystal Structure of Frameshift Suppressor tRNA SufA6 Bound to Codon CCG-G on the Ribosome
Authors : Maehigashi, T.; Dunkle, J.A.; Dunham, C.M.
Deposited on : 2013-06-25
Resolution : 3.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	FAILED
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

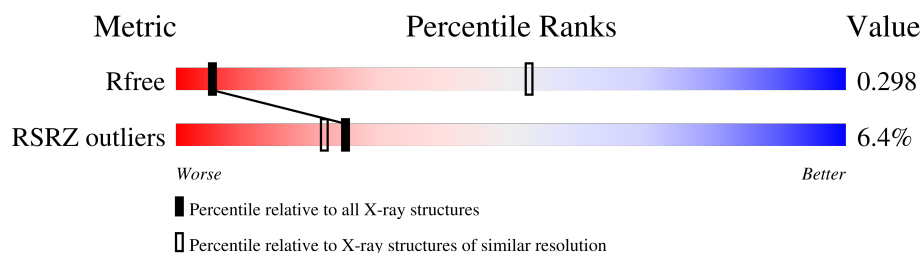
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1270 (4.10-3.70)
RSRZ outliers	180081	1269 (4.10-3.70)

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	QV	101	-	-	-	X
57	MG	RA	3006	-	-	-	X
57	MG	RA	3012	-	-	-	X
57	MG	RA	3018	-	-	-	X
57	MG	RA	3026	-	-	-	X
57	MG	RA	3032	-	-	-	X
57	MG	RA	3033	-	-	-	X
57	MG	RA	3065	-	-	-	X
57	MG	RA	3094	-	-	-	X
57	MG	RA	3097	-	-	-	X
57	MG	RA	3100	-	-	-	X
57	MG	RA	3232	-	-	-	X
57	MG	RP	201	-	-	-	X
57	MG	XA	1601	-	-	-	X
57	MG	YA	3002	-	-	-	X
57	MG	YA	3012	-	-	-	X
57	MG	YA	3025	-	-	-	X
57	MG	YA	3031	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	YA	3033	-	-	-	X
57	MG	YA	3035	-	-	-	X
57	MG	YA	3050	-	-	-	X
57	MG	YA	3054	-	-	-	X
57	MG	YA	3088	-	-	-	X
57	MG	YA	3103	-	-	-	X
57	MG	YA	3109	-	-	-	X
57	MG	YA	3258	-	-	-	X
57	MG	YD	301	-	-	-	X

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 291958 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	QA	1500	Total	C	N	O	P	0	0	0
			32247	14353	5981	10414	1499			
1	XA	1500	Total	C	N	O	P	0	0	0
			32249	14354	5984	10412	1499			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	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			

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	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 S21.

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 fMet.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	QV	77	Total	C	N	O	P	0	0	0
			1644	732	297	538	77			
22	XV	77	Total	C	N	O	P	0	0	0
			1644	732	297	538	77			

- Molecule 23 is a RNA chain called A-site ASL SufA6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QX	8	Total	C	N	O	P	0	0	0
			173	77	33	55	8			
23	XX	8	Total	C	N	O	P	0	0	0
			173	77	33	55	8			

- Molecule 24 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	QY	14	Total	C	N	O	P	0	0	0
			303	135	55	99	14			
24	XY	14	Total	C	N	O	P	0	0	0
			303	135	55	99	14			

- Molecule 25 is a RNA chain called 23S rRNA.

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

- Molecule 26 is a RNA chain called 5S rRNA.

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

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

- Molecule 27 is a protein called 50S ribosomal protein L2.

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

- Molecule 28 is a protein called 50S ribosomal protein L3.

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

- Molecule 29 is a protein called 50S ribosomal protein L4.

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

- Molecule 30 is a protein called 50S ribosomal protein L5.

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

- Molecule 31 is a protein called 50S ribosomal protein L6.

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

- Molecule 32 is a protein called 50S ribosomal protein L9.

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

- Molecule 33 is a protein called 50S ribosomal protein L13.

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

- Molecule 34 is a protein called 50S ribosomal protein L14.

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

- Molecule 35 is a protein called 50S ribosomal protein L15.

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

- Molecule 36 is a protein called 50S ribosomal protein L16.

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

- Molecule 37 is a protein called 50S ribosomal protein L17.

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

- Molecule 38 is a protein called 50S ribosomal protein L18.

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

- Molecule 39 is a protein called 50S ribosomal protein L19.

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

- Molecule 40 is a protein called 50S ribosomal protein L20.

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

- Molecule 41 is a protein called 50S ribosomal protein L21.

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

- Molecule 42 is a protein called 50S ribosomal protein L22.

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

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

- Molecule 43 is a protein called 50S ribosomal protein L23.

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

- Molecule 44 is a protein called 50S ribosomal protein L24.

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

- Molecule 45 is a protein called 50S ribosomal protein L25.

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

- Molecule 46 is a protein called 50S ribosomal protein L27.

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

- Molecule 47 is a protein called 50S ribosomal protein L28.

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

- Molecule 48 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	R2	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			
48	Y2	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			

- Molecule 49 is a protein called 50S ribosomal protein L30.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L32.

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

- Molecule 52 is a protein called 50S ribosomal protein L33.

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

- Molecule 53 is a protein called 50S ribosomal protein L34.

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

- Molecule 54 is a protein called 50S ribosomal protein L35.

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

- Molecule 55 is a protein called 50S ribosomal protein L36.

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

- Molecule 56 is a RNA chain called tRNA acceptor end mimic.

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).

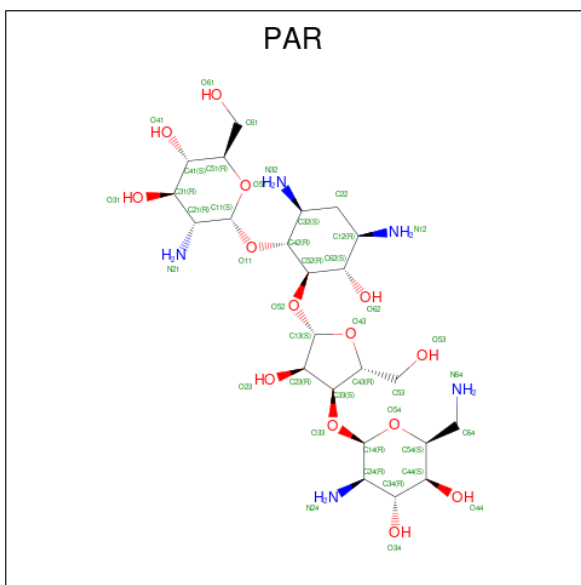
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QA	65	Total	Mg	0	0
			65	65		
57	QF	1	Total	Mg	0	0
			1	1		
57	QM	1	Total	Mg	0	0
			1	1		
57	QV	1	Total	Mg	0	0
			1	1		
57	RA	242	Total	Mg	0	0
			242	242		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	RB	2	Total 2	Mg 2	0	0
57	RD	1	Total 1	Mg 1	0	0
57	RE	2	Total 2	Mg 2	0	0
57	RF	1	Total 1	Mg 1	0	0
57	RP	2	Total 2	Mg 2	0	0
57	R0	1	Total 1	Mg 1	0	0
57	R5	1	Total 1	Mg 1	0	0
57	R8	1	Total 1	Mg 1	0	0
57	XA	70	Total 70	Mg 70	0	0
57	XB	1	Total 1	Mg 1	0	0
57	XM	1	Total 1	Mg 1	0	0
57	XV	1	Total 1	Mg 1	0	0
57	XX	1	Total 1	Mg 1	0	0
57	YA	267	Total 267	Mg 267	0	0
57	YB	3	Total 3	Mg 3	0	0
57	YD	2	Total 2	Mg 2	0	0
57	YE	1	Total 1	Mg 1	0	0
57	YP	1	Total 1	Mg 1	0	0
57	Y0	1	Total 1	Mg 1	0	0

- Molecule 58 is PAROMOMYCIN (CCD ID: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
58	QA	1	Total 42	C 23	N 5	O 14	0	0
58	XA	1	Total 42	C 23	N 5	O 14	0	0

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

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

MolProbit 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	209.03Å 447.05Å 619.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.88 – 3.90 49.88 – 3.90	Depositor EDS
% Data completeness (in resolution range)	97.9 (49.88-3.90) 97.9 (49.88-3.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 3.57Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.252 , 0.298 0.252 , 0.298	Depositor DCC
R_{free} test set	29573 reflections (4.55%)	wwPDB-VP
Wilson B-factor (Å ²)	100.8	Xtriage
Anisotropy	0.363	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 54.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	291958	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.51% 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](#)

4 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	$\# Z > 2$
24	1MG	QY	37	24	23,26,27	2.45	4 (17%)	33,39,42	2.05	7 (21%)
56	PPU	Z6	76	56,25	37,40,41	2.58	8 (21%)	47,57,60	2.57	15 (31%)
56	PPU	Z8	76	56,25	37,40,41	2.57	8 (21%)	47,57,60	2.56	15 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	1MG	XY	37	24	23,26,27	2.46	4 (17%)	33,39,42	2.04	8 (24%)

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
24	1MG	QY	37	24	-	0/7/25/26	0/3/3/3
56	PPU	Z6	76	56,25	-	2/25/43/44	0/4/4/4
56	PPU	Z8	76	56,25	-	2/25/43/44	0/4/4/4
24	1MG	XY	37	24	-	0/7/25/26	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	Z8	76	PPU	O-C	9.58	1.41	1.23
56	Z6	76	PPU	O-C	9.57	1.41	1.23
24	XY	37	1MG	C2-N2	7.71	1.47	1.34
24	QY	37	1MG	C2-N2	7.65	1.47	1.34
24	XY	37	1MG	C4-N3	6.64	1.49	1.34
24	QY	37	1MG	C4-N3	6.59	1.49	1.34
56	Z6	76	PPU	C9-N6	-6.22	1.32	1.45
56	Z8	76	PPU	C9-N6	-6.16	1.32	1.45
56	Z6	76	PPU	C-N3'	5.93	1.46	1.34
56	Z6	76	PPU	C10-N6	-5.88	1.32	1.45
56	Z8	76	PPU	C10-N6	-5.88	1.32	1.45
56	Z8	76	PPU	C-N3'	5.83	1.46	1.34
24	QY	37	1MG	C2-N1	4.54	1.45	1.37
24	XY	37	1MG	C2-N1	4.53	1.45	1.37
56	Z8	76	PPU	C5-N7	-3.53	1.32	1.39
56	Z6	76	PPU	C5-N7	-3.51	1.32	1.39
56	Z6	76	PPU	C8-N9	-3.28	1.32	1.37
56	Z8	76	PPU	C8-N9	-3.15	1.32	1.37
56	Z8	76	PPU	C1'-N9	2.74	1.53	1.46
56	Z6	76	PPU	C1'-N9	2.71	1.53	1.46
24	QY	37	1MG	C5-N7	-2.51	1.34	1.39
24	XY	37	1MG	C5-N7	-2.48	1.34	1.39
56	Z6	76	PPU	C4-N9	-2.18	1.33	1.37
56	Z8	76	PPU	C4-N9	-2.12	1.33	1.37

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	Z6	76	PPU	C3'-N3'-C	-8.59	110.13	123.20
56	Z8	76	PPU	C3'-N3'-C	-8.54	110.21	123.20
24	QY	37	1MG	N2-C2-N1	6.35	123.89	118.79
24	XY	37	1MG	N2-C2-N1	6.29	123.84	118.79
56	Z8	76	PPU	C2'-C1'-N9	-5.97	98.48	113.30
56	Z6	76	PPU	C2'-C1'-N9	-5.94	98.55	113.30
56	Z6	76	PPU	C5-C4-N3	-5.08	119.72	126.72
56	Z8	76	PPU	C5-C4-N3	-4.98	119.86	126.72
56	Z8	76	PPU	N3-C2-N1	-4.76	121.38	128.58
56	Z6	76	PPU	N3-C2-N1	-4.76	121.38	128.58
24	XY	37	1MG	C5-C4-N3	-4.73	120.87	128.39
24	QY	37	1MG	C5-C4-N3	-4.69	120.92	128.39
56	Z6	76	PPU	C2-N1-C6	4.08	121.80	111.83
56	Z8	76	PPU	CA-C-N3'	4.06	121.71	116.21
56	Z8	76	PPU	C2-N1-C6	4.06	121.75	111.83
56	Z6	76	PPU	C4-C5-N7	-4.04	105.96	110.58
56	Z6	76	PPU	CA-C-N3'	4.03	121.67	116.21
56	Z8	76	PPU	C4-C5-N7	-4.00	106.01	110.58
24	QY	37	1MG	C2-N3-C4	3.84	120.61	111.98
24	XY	37	1MG	C2-N3-C4	3.82	120.58	111.98
56	Z6	76	PPU	C2-N3-C4	3.71	120.90	111.83
56	Z8	76	PPU	C2-N3-C4	3.68	120.83	111.83
56	Z8	76	PPU	C5-N7-C8	3.55	109.02	103.45
24	XY	37	1MG	N9-C4-N3	3.53	133.01	125.95
56	Z6	76	PPU	C5-N7-C8	3.53	108.99	103.45
24	QY	37	1MG	N9-C4-N3	3.52	132.99	125.95
24	QY	37	1MG	C2-N1-C6	3.51	123.92	120.99
56	Z8	76	PPU	CM-OC-CZ	-3.41	110.18	117.50
56	Z6	76	PPU	CM-OC-CZ	-3.41	110.18	117.50
56	Z8	76	PPU	N9-C8-N7	-3.36	109.16	113.94
24	XY	37	1MG	C2-N1-C6	3.36	123.79	120.99
56	Z6	76	PPU	N9-C8-N7	-3.35	109.19	113.94
56	Z8	76	PPU	O4'-C1'-N9	-3.01	102.31	108.09
56	Z6	76	PPU	O4'-C1'-N9	-3.00	102.33	108.09
56	Z6	76	PPU	N3-C4-N9	2.96	132.20	127.17
56	Z8	76	PPU	N3-C4-N9	2.85	132.01	127.17
24	XY	37	1MG	C8-N7-C5	2.68	109.04	104.26
24	QY	37	1MG	C8-N7-C5	2.64	108.97	104.26
56	Z6	76	PPU	C4-C5-C6	2.50	118.50	115.91
56	Z8	76	PPU	C4-C5-C6	2.45	118.44	115.91
56	Z8	76	PPU	C5-C4-N9	2.13	108.14	105.81
24	XY	37	1MG	C6-C5-N7	2.13	134.08	129.36
24	QY	37	1MG	C6-C5-N7	2.08	133.98	129.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	Z6	76	PPU	C5-C4-N9	2.08	108.08	105.81
24	XY	37	1MG	C4-C5-N7	-2.02	107.47	110.67

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	Z6	76	PPU	O-C-CA-N
56	Z8	76	PPU	O-C-CA-N
56	Z6	76	PPU	N3'-C-CA-N
56	Z8	76	PPU	N3'-C-CA-N

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 676 ligands modelled in this entry, 674 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	PAR	QA	1666	-	44,45,45	1.37	8 (18%)	63,67,67	1.46	10 (15%)
58	PAR	XA	1671	-	44,45,45	1.56	8 (18%)	63,67,67	1.82	16 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	PAR	QA	1666	-	-	6/18/94/94	0/4/4/4
58	PAR	XA	1671	-	-	4/18/94/94	0/4/4/4

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	XA	1671	PAR	C31-C21	4.76	1.59	1.53
58	XA	1671	PAR	C11-C21	3.81	1.59	1.52
58	QA	1666	PAR	C52-C42	2.97	1.58	1.52
58	XA	1671	PAR	O54-C14	2.83	1.49	1.41
58	XA	1671	PAR	C52-C42	2.78	1.58	1.52
58	XA	1671	PAR	C62-C52	2.75	1.59	1.52
58	QA	1666	PAR	O51-C11	2.71	1.48	1.41
58	QA	1666	PAR	C11-C21	2.69	1.57	1.52
58	QA	1666	PAR	C62-C52	2.43	1.58	1.52
58	QA	1666	PAR	O54-C14	2.39	1.48	1.41
58	XA	1671	PAR	C14-C24	2.38	1.57	1.52
58	XA	1671	PAR	O51-C11	2.29	1.47	1.41
58	XA	1671	PAR	C44-C34	2.28	1.58	1.52
58	QA	1666	PAR	C44-C54	2.26	1.57	1.53
58	QA	1666	PAR	O54-C54	2.18	1.49	1.44
58	QA	1666	PAR	C44-C34	2.10	1.57	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	XA	1671	PAR	O33-C14-C24	5.19	116.57	108.08
58	XA	1671	PAR	C32-C22-C12	-4.65	103.05	111.02
58	QA	1666	PAR	O54-C54-C64	4.45	114.61	106.07
58	QA	1666	PAR	C14-O54-C54	3.48	120.52	113.72
58	XA	1671	PAR	O54-C54-C64	3.47	112.75	106.07
58	XA	1671	PAR	O41-C41-C51	3.26	117.35	109.32
58	XA	1671	PAR	C14-O54-C54	3.26	120.08	113.72
58	QA	1666	PAR	C41-C31-C21	-3.18	105.71	110.99
58	XA	1671	PAR	O31-C31-C21	3.11	115.81	110.22
58	XA	1671	PAR	C11-C21-C31	3.04	117.90	110.29
58	XA	1671	PAR	O34-C34-C24	-2.94	104.94	110.22
58	QA	1666	PAR	O33-C14-C24	2.74	112.57	108.08
58	QA	1666	PAR	C44-C34-C24	2.73	115.53	110.99
58	XA	1671	PAR	C31-C41-C51	-2.72	105.30	110.23
58	XA	1671	PAR	O11-C11-C21	2.72	112.53	108.08
58	QA	1666	PAR	C11-C21-N21	2.66	114.99	110.20
58	XA	1671	PAR	C52-C62-C12	2.66	116.34	109.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	XA	1671	PAR	C11-O11-C42	2.63	124.21	117.98
58	XA	1671	PAR	O62-C62-C12	-2.62	105.00	109.90
58	QA	1666	PAR	C11-O51-C51	2.55	118.70	113.72
58	XA	1671	PAR	C62-C52-C42	2.52	117.38	111.72
58	QA	1666	PAR	C32-C22-C12	-2.44	106.84	111.02
58	QA	1666	PAR	O33-C14-O54	-2.39	104.41	110.69
58	XA	1671	PAR	C52-C42-C32	-2.37	106.92	111.31
58	QA	1666	PAR	O11-C42-C32	-2.16	104.03	109.18
58	XA	1671	PAR	O54-C54-C44	-2.09	105.93	109.70

There are no chirality outliers.

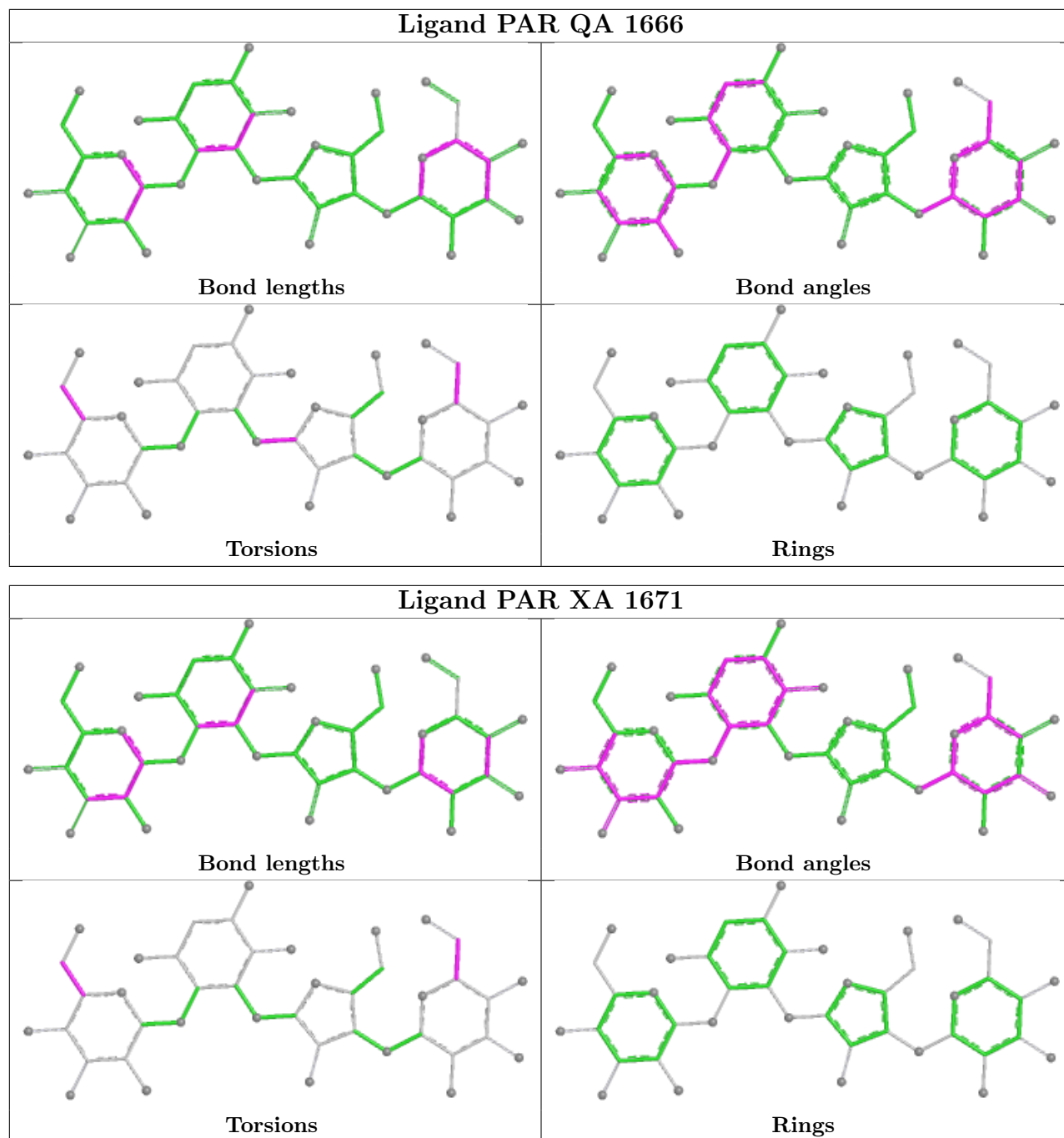
All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	QA	1666	PAR	C44-C54-C64-N64
58	QA	1666	PAR	O54-C54-C64-N64
58	XA	1671	PAR	C44-C54-C64-N64
58	XA	1671	PAR	O54-C54-C64-N64
58	XA	1671	PAR	O51-C51-C61-O61
58	QA	1666	PAR	O51-C51-C61-O61
58	XA	1671	PAR	C41-C51-C61-O61
58	QA	1666	PAR	C41-C51-C61-O61
58	QA	1666	PAR	C23-C13-O52-C52
58	QA	1666	PAR	O43-C13-O52-C52

There are no ring outliers.

No monomer is involved in short contacts.

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



4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data ⓘ

5.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	QA	1500/1522 (98%)	0.17	41 (2%) 56 39	35, 87, 182, 299	0
1	XA	1500/1522 (98%)	0.01	23 (1%) 72 50	21, 74, 169, 271	0
2	QB	237/256 (92%)	0.45	11 (4%) 37 28	84, 154, 204, 236	0
2	XB	237/256 (92%)	0.33	14 (5%) 28 24	51, 121, 182, 226	0
3	QC	205/239 (85%)	0.55	15 (7%) 21 19	57, 135, 182, 201	0
3	XC	205/239 (85%)	0.25	10 (4%) 35 27	32, 89, 145, 177	0
4	QD	208/209 (99%)	0.90	30 (14%) 6 9	38, 99, 165, 221	0
4	XD	208/209 (99%)	0.78	16 (7%) 19 18	27, 106, 160, 186	0
5	QE	151/162 (93%)	0.66	10 (6%) 24 21	36, 111, 158, 185	0
5	XE	151/162 (93%)	0.49	9 (5%) 27 23	3, 85, 142, 170	0
6	QF	101/101 (100%)	0.32	3 (2%) 52 36	33, 99, 158, 181	0
6	XF	101/101 (100%)	0.42	7 (6%) 23 20	25, 95, 145, 243	0
7	QG	155/156 (99%)	0.56	10 (6%) 25 22	55, 123, 179, 210	0
7	XG	155/156 (99%)	0.23	5 (3%) 50 35	42, 99, 156, 197	0
8	QH	138/138 (100%)	0.89	18 (13%) 7 10	61, 120, 167, 193	0
8	XH	138/138 (100%)	0.65	10 (7%) 21 20	20, 94, 147, 198	0
9	QI	127/128 (99%)	0.99	21 (16%) 4 7	67, 134, 193, 224	0
9	XI	127/128 (99%)	0.95	17 (13%) 7 10	29, 107, 165, 195	0
10	QJ	99/105 (94%)	1.24	16 (16%) 4 7	46, 149, 202, 222	0
10	XJ	99/105 (94%)	0.85	14 (14%) 6 9	35, 115, 175, 201	0
11	QK	119/129 (92%)	0.78	14 (11%) 9 12	42, 104, 158, 202	0
11	XK	119/129 (92%)	0.63	7 (5%) 28 24	27, 87, 148, 170	0
12	QL	125/132 (94%)	1.14	25 (20%) 3 5	21, 93, 142, 192	0
12	XL	125/132 (94%)	0.97	20 (16%) 5 8	20, 66, 131, 212	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
13	QM	121/126 (96%)	0.83	15 (12%)	8 11	58, 122, 175, 214	0
13	XM	121/126 (96%)	0.65	11 (9%)	15 16	28, 92, 144, 180	0
14	QN	60/61 (98%)	1.06	10 (16%)	4 7	55, 129, 181, 204	0
14	XN	60/61 (98%)	1.03	9 (15%)	5 8	33, 82, 135, 170	0
15	QO	88/89 (98%)	0.60	7 (7%)	18 18	54, 105, 154, 178	0
15	XO	88/89 (98%)	0.59	7 (7%)	18 18	25, 91, 141, 171	0
16	QP	84/88 (95%)	1.13	16 (19%)	3 5	42, 86, 157, 171	0
16	XP	84/88 (95%)	1.10	13 (15%)	5 8	51, 101, 152, 235	0
17	QQ	100/105 (95%)	0.97	14 (14%)	6 9	33, 91, 144, 165	0
17	XQ	100/105 (95%)	0.84	12 (12%)	9 12	37, 95, 147, 200	0
18	QR	70/88 (79%)	0.31	0	100 100	42, 110, 160, 212	0
18	XR	70/88 (79%)	0.38	1 (1%)	73 52	34, 86, 147, 168	0
19	QS	84/93 (90%)	0.85	10 (11%)	9 12	60, 131, 184, 190	0
19	XS	84/93 (90%)	0.84	8 (9%)	14 16	45, 97, 141, 220	0
20	QT	99/106 (93%)	0.71	14 (14%)	6 9	34, 91, 154, 181	0
20	XT	99/106 (93%)	1.10	22 (22%)	2 4	50, 112, 158, 181	0
21	QU	25/27 (92%)	1.89	10 (40%)	1 1	62, 132, 185, 206	0
21	XU	25/27 (92%)	2.17	11 (44%)	0 1	45, 89, 136, 166	0
22	QV	77/77 (100%)	0.51	2 (2%)	57 40	26, 99, 158, 205	0
22	XV	77/77 (100%)	0.29	2 (2%)	57 40	28, 70, 121, 185	0
23	QX	8/25 (32%)	2.22	3 (37%)	1 2	70, 95, 129, 169	0
23	XX	8/25 (32%)	1.83	2 (25%)	2 4	36, 51, 102, 163	0
24	QY	13/18 (72%)	1.44	3 (23%)	2 4	104, 150, 249, 294	0
24	XY	13/18 (72%)	1.07	1 (7%)	19 18	70, 106, 221, 249	0
25	RA	2882/2916 (98%)	-0.03	49 (1%)	69 48	14, 60, 203, 320	0
25	YA	2883/2916 (98%)	-0.09	35 (1%)	76 55	14, 50, 194, 329	0
26	RB	120/122 (98%)	0.32	1 (0%)	82 64	64, 113, 177, 203	0
26	YB	120/122 (98%)	-0.17	1 (0%)	82 64	37, 69, 95, 158	0
27	RD	272/276 (98%)	0.77	37 (13%)	7 10	7, 56, 113, 177	0
27	YD	272/276 (98%)	0.56	21 (7%)	19 18	3, 49, 98, 152	0
28	RE	205/206 (99%)	0.82	24 (11%)	9 12	23, 73, 150, 195	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
28	YE	205/206 (99%)	0.71	18 (8%)	15 17	15, 77, 151, 200	0
29	RF	202/210 (96%)	0.55	11 (5%)	31 25	4, 85, 151, 184	0
29	YF	202/210 (96%)	0.52	12 (5%)	28 24	8, 65, 124, 184	0
30	RG	181/182 (99%)	0.82	24 (13%)	7 10	52, 137, 205, 232	0
30	YG	181/182 (99%)	0.66	11 (6%)	27 23	25, 98, 166, 203	0
31	RH	170/180 (94%)	0.74	20 (11%)	9 12	69, 150, 202, 250	0
31	YH	170/180 (94%)	0.76	15 (8%)	15 17	32, 94, 152, 204	0
32	RI	146/148 (98%)	0.48	7 (4%)	35 27	29, 108, 161, 182	0
32	YI	146/148 (98%)	0.20	3 (2%)	63 44	18, 95, 158, 203	0
33	RN	138/140 (98%)	0.88	22 (15%)	5 8	33, 94, 152, 192	0
33	YN	138/140 (98%)	0.72	14 (10%)	12 15	19, 75, 132, 162	0
34	RO	122/122 (100%)	0.52	8 (6%)	24 21	6, 64, 120, 163	0
34	YO	122/122 (100%)	0.63	8 (6%)	24 21	18, 60, 114, 144	0
35	RP	150/150 (100%)	0.88	17 (11%)	10 13	5, 87, 160, 191	0
35	YP	150/150 (100%)	0.97	20 (13%)	7 10	17, 75, 166, 203	0
36	RQ	141/141 (100%)	0.92	15 (10%)	11 14	25, 94, 140, 212	0
36	YQ	141/141 (100%)	0.81	15 (10%)	11 14	11, 61, 126, 169	0
37	RR	118/118 (100%)	0.63	6 (5%)	33 26	12, 58, 116, 154	0
37	YR	118/118 (100%)	0.93	19 (16%)	4 7	24, 68, 127, 155	0
38	RS	111/112 (99%)	0.80	12 (10%)	11 14	40, 116, 169, 194	0
38	YS	111/112 (99%)	0.42	11 (9%)	13 15	9, 79, 133, 232	0
39	RT	137/146 (93%)	0.43	4 (2%)	53 37	19, 77, 171, 214	0
39	YT	137/146 (93%)	0.75	13 (9%)	14 16	30, 84, 164, 206	0
40	RU	117/118 (99%)	0.66	8 (6%)	23 21	17, 78, 154, 194	0
40	YU	117/118 (99%)	0.59	7 (5%)	27 23	15, 65, 152, 189	0
41	RV	101/101 (100%)	0.49	12 (11%)	9 12	36, 105, 157, 216	0
41	YV	101/101 (100%)	0.50	4 (3%)	42 31	23, 84, 144, 243	0
42	RW	113/113 (100%)	0.58	6 (5%)	32 25	20, 65, 137, 216	0
42	YW	113/113 (100%)	0.54	9 (7%)	18 18	12, 56, 114, 193	0
43	RX	92/96 (95%)	0.81	7 (7%)	20 19	14, 69, 125, 158	0
43	YX	92/96 (95%)	0.80	8 (8%)	16 17	12, 56, 113, 138	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	RY	102/110 (92%)	1.45	25 (24%) 2 4	36, 115, 175, 230	0
44	YY	102/110 (92%)	0.84	14 (13%) 6 10	24, 83, 156, 204	0
45	RZ	183/206 (88%)	0.41	3 (1%) 70 49	42, 122, 174, 213	0
45	YZ	183/206 (88%)	0.44	8 (4%) 39 29	23, 98, 153, 211	0
46	R0	82/85 (96%)	0.58	6 (7%) 21 19	13, 74, 111, 143	0
46	Y0	82/85 (96%)	0.11	1 (1%) 76 55	11, 54, 85, 133	0
47	R1	97/98 (98%)	1.19	18 (18%) 3 6	11, 74, 170, 241	0
47	Y1	97/98 (98%)	0.89	17 (17%) 4 6	11, 64, 144, 205	0
48	R2	69/72 (95%)	0.75	6 (8%) 16 17	26, 101, 176, 197	0
48	Y2	69/72 (95%)	0.79	9 (13%) 7 10	26, 69, 141, 177	0
49	R3	59/60 (98%)	1.01	7 (11%) 9 12	19, 95, 150, 200	0
49	Y3	59/60 (98%)	0.74	4 (6%) 23 21	9, 70, 131, 166	0
50	R4	71/71 (100%)	0.66	5 (7%) 22 20	89, 171, 218, 267	0
50	Y4	71/71 (100%)	0.69	3 (4%) 40 30	69, 145, 208, 248	0
51	R5	59/60 (98%)	0.72	5 (8%) 16 17	13, 74, 179, 222	0
51	Y5	59/60 (98%)	0.69	7 (11%) 9 12	17, 78, 189, 225	0
52	R6	49/54 (90%)	0.90	4 (8%) 17 18	101, 150, 215, 233	0
52	Y6	49/54 (90%)	0.80	3 (6%) 27 23	73, 147, 211, 217	0
53	R7	49/49 (100%)	0.80	7 (14%) 6 9	17, 47, 108, 188	0
53	Y7	49/49 (100%)	0.71	6 (12%) 8 12	6, 40, 118, 133	0
54	R8	64/65 (98%)	1.54	20 (31%) 1 3	24, 80, 155, 197	0
54	Y8	64/65 (98%)	1.23	14 (21%) 2 4	6, 54, 120, 197	0
55	R9	37/37 (100%)	2.30	18 (48%) 0 1	94, 143, 197, 202	0
55	Y9	37/37 (100%)	3.07	27 (72%) 0 0	62, 123, 202, 228	0
56	Z6	2/3 (66%)	0.27	0 100 100	30, 30, 30, 75	0
56	Z8	2/3 (66%)	0.05	0 100 100	30, 30, 30, 47	0
All	All	20871/21494 (97%)	0.40	1340 (6%) 25 22	3, 80, 177, 329	0

All (1340) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	QK	129	SER	12.1
11	XK	129	SER	9.7

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Mol	Chain	Res	Type	RSRZ
9	XI	8	GLY	9.5
53	R7	49	ARG	9.5
10	QJ	58	ASP	9.5
54	R8	54	GLU	8.5
12	QL	19	ARG	7.7
23	XX	8	A	7.6
5	XE	81	GLU	7.3
11	XK	127	LYS	7.1
55	R9	22	ARG	7.1
54	Y8	3	LYS	6.8
36	RQ	80	GLU	6.8
53	Y7	48	LYS	6.8
55	Y9	21	GLY	6.7
36	RQ	12	GLN	6.6
21	XU	10	ARG	6.6
44	RY	22	GLY	6.5
35	RP	16	ARG	6.4
55	Y9	26	ILE	6.3
20	XT	9	ASN	6.3
8	XH	1	MET	6.2
11	QK	128	ALA	6.2
5	QE	20	GLN	6.1
28	YE	204	ALA	6.1
55	R9	11	CYS	6.1
55	Y9	1	MET	6.1
44	RY	24	VAL	6.0
47	Y1	98	LEU	6.0
14	XN	2	ALA	5.9
11	XK	128	ALA	5.8
55	R9	26	ILE	5.8
44	RY	62	GLU	5.7
39	YT	106	SER	5.7
53	Y7	49	ARG	5.7
30	RG	157	ILE	5.6
55	Y9	25	VAL	5.5
20	XT	23	ARG	5.5
39	YT	21	GLU	5.4
44	YY	71	LYS	5.4
9	QI	26	VAL	5.4
36	RQ	79	LEU	5.4
55	R9	28	GLU	5.4
13	QM	102	ARG	5.3

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Mol	Chain	Res	Type	RSRZ
2	QB	163	PHE	5.3
54	R8	56	GLU	5.3
21	XU	15	ARG	5.3
9	XI	41	VAL	5.2
21	QU	2	GLY	5.2
51	R5	2	ALA	5.2
10	QJ	98	ILE	5.2
40	RU	56	ASP	5.2
7	QG	5	ARG	5.2
8	QH	1	MET	5.2
48	Y2	69	ARG	5.2
10	QJ	59	SER	5.1
12	XL	28	LYS	5.1
36	YQ	80	GLU	5.1
44	RY	45	VAL	5.1
35	YP	114	ILE	5.0
12	QL	32	PHE	5.0
21	XU	26	LYS	5.0
13	QM	88	ARG	5.0
21	QU	16	GLY	5.0
20	XT	21	LYS	5.0
25	RA	2062	A	5.0
48	Y2	71	ASN	4.9
12	XL	23	LYS	4.9
25	RA	1061	U	4.9
9	XI	127	LYS	4.9
12	XL	89	ARG	4.9
14	XN	41	ARG	4.9
20	XT	18	GLN	4.9
27	YD	236	GLY	4.8
44	RY	94	LYS	4.8
12	XL	19	ARG	4.8
3	XC	158	GLY	4.8
23	QX	8	A	4.8
30	RG	142	PRO	4.8
47	R1	70	VAL	4.7
13	XM	94	ARG	4.7
35	YP	64	LYS	4.7
44	RY	16	ALA	4.7
45	YZ	113	ALA	4.7
20	QT	66	ALA	4.7
51	Y5	3	LYS	4.7

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Mol	Chain	Res	Type	RSRZ
55	Y9	16	VAL	4.7
10	QJ	4	ILE	4.7
10	QJ	60	ARG	4.6
17	QQ	58	GLU	4.6
49	Y3	55	ARG	4.6
34	RO	32	TYR	4.6
55	Y9	18	ARG	4.6
5	XE	21	ALA	4.5
39	YT	1	MET	4.5
7	QG	108	ALA	4.5
8	QH	4	ASP	4.5
37	RR	5	LYS	4.5
5	QE	81	GLU	4.5
13	XM	111	LYS	4.5
25	RA	1060	U	4.5
41	YV	71	LEU	4.4
55	Y9	28	GLU	4.4
7	QG	4	ARG	4.4
10	XJ	59	SER	4.4
50	R4	69	LYS	4.4
55	Y9	8	LYS	4.4
21	XU	2	GLY	4.4
41	RV	81	TYR	4.4
4	QD	67	ILE	4.4
11	QK	127	LYS	4.4
35	RP	18	ARG	4.4
20	XT	11	SER	4.4
4	QD	5	ILE	4.4
20	QT	21	LYS	4.4
38	YS	2	ALA	4.4
16	XP	22	THR	4.4
12	XL	7	ILE	4.3
9	QI	123	PRO	4.3
47	R1	98	LEU	4.3
13	QM	100	GLY	4.3
25	YA	614	U	4.3
21	QU	15	ARG	4.3
13	QM	75	ALA	4.3
12	QL	23	LYS	4.3
14	QN	29	ARG	4.3
35	YP	16	ARG	4.3
55	R9	37	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
31	RH	171	LEU	4.3
36	YQ	5	ARG	4.2
54	R8	64	TYR	4.2
3	XC	159	GLY	4.2
27	YD	40	THR	4.2
44	RY	79	CYS	4.2
16	XP	66	PRO	4.2
25	YA	1177	A	4.2
16	XP	15	PRO	4.2
54	R8	59	LYS	4.2
3	QC	91	LEU	4.2
55	Y9	23	VAL	4.2
14	QN	41	ARG	4.2
30	RG	34	LEU	4.2
45	YZ	28	MET	4.1
55	R9	12	ASP	4.1
12	QL	96	VAL	4.1
54	R8	61	LEU	4.1
52	R6	42	TRP	4.1
12	QL	72	GLY	4.1
47	R1	10	LYS	4.1
16	QP	61	SER	4.1
8	QH	101	PRO	4.1
46	R0	71	ASP	4.1
44	RY	14	LEU	4.1
4	QD	3	ARG	4.1
52	Y6	23	THR	4.1
11	XK	117	ASN	4.1
49	Y3	56	VAL	4.0
4	QD	50	ARG	4.0
55	Y9	4	ARG	4.0
12	XL	120	TYR	4.0
3	QC	158	GLY	4.0
7	QG	81	GLY	4.0
50	Y4	66	SER	4.0
53	Y7	45	ALA	4.0
41	RV	74	LYS	4.0
12	XL	27	LEU	4.0
4	QD	209	ARG	4.0
16	XP	28	ARG	4.0
9	XI	110	GLU	4.0
40	YU	13	LYS	4.0

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Mol	Chain	Res	Type	RSRZ
4	QD	49	ARG	4.0
34	YO	38	VAL	4.0
9	QI	62	TYR	4.0
54	R8	55	ALA	4.0
33	RN	40	PRO	4.0
55	Y9	15	LYS	3.9
3	QC	87	LEU	3.9
51	Y5	57	VAL	3.9
38	YS	8	GLU	3.9
7	XG	5	ARG	3.9
20	QT	75	ASN	3.9
28	YE	76	ARG	3.9
55	R9	35	ARG	3.9
17	XQ	36	ILE	3.9
27	RD	38	LYS	3.9
34	RO	1	MET	3.9
23	QX	7	G	3.9
27	YD	176	ARG	3.9
30	RG	159	VAL	3.9
25	YA	2062	A	3.9
12	QL	31	PRO	3.9
12	QL	71	PRO	3.9
47	R1	92	LYS	3.9
14	QN	25	VAL	3.9
25	YA	2116	G	3.9
35	RP	14	LYS	3.9
38	RS	13	ARG	3.9
45	RZ	83	PRO	3.9
19	XS	11	VAL	3.9
48	R2	52	ASP	3.9
41	RV	78	LYS	3.9
9	QI	127	LYS	3.8
17	XQ	100	LYS	3.8
25	RA	1059	G	3.8
54	Y8	9	GLY	3.8
33	YN	138	LEU	3.8
25	YA	988	A	3.8
3	QC	167	TRP	3.8
48	Y2	70	GLN	3.8
54	Y8	65	GLU	3.8
20	XT	68	LYS	3.8
27	RD	5	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
16	XP	25	ARG	3.8
14	QN	46	GLU	3.8
3	XC	167	TRP	3.8
20	QT	72	LEU	3.8
41	YV	84	LYS	3.8
44	RY	33	LYS	3.8
29	RF	78	ILE	3.8
31	YH	144	VAL	3.8
39	YT	104	ASN	3.7
44	YY	46	LYS	3.7
9	QI	41	VAL	3.7
36	YQ	91	GLU	3.7
19	XS	78	ARG	3.7
16	QP	56	ALA	3.7
46	R0	2	ALA	3.7
55	R9	15	LYS	3.7
31	YH	171	LEU	3.7
47	Y1	70	VAL	3.7
2	XB	134	GLU	3.7
43	RX	38	GLU	3.7
9	QI	27	THR	3.7
13	QM	61	GLU	3.7
1	QA	1202	G	3.7
27	YD	39	LYS	3.7
17	QQ	7	THR	3.6
20	XT	29	LYS	3.6
13	QM	101	GLN	3.6
55	Y9	17	ILE	3.6
53	Y7	1	MET	3.6
20	XT	70	SER	3.6
12	XL	98	TYR	3.6
13	XM	102	ARG	3.6
38	RS	2	ALA	3.6
53	R7	47	ARG	3.6
55	Y9	9	ARG	3.6
31	YH	155	SER	3.6
27	RD	36	PRO	3.6
52	Y6	42	TRP	3.6
1	QA	328	C	3.6
13	XM	115	LYS	3.6
22	QV	1	C	3.6
38	YS	93	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
48	R2	8	LYS	3.6
10	XJ	47	PHE	3.6
9	XI	105	ASP	3.6
40	YU	97	ASP	3.6
55	Y9	34	GLN	3.6
17	XQ	32	TYR	3.6
20	QT	30	LYS	3.6
16	QP	28	ARG	3.6
21	XU	6	ARG	3.5
27	RD	217	ARG	3.5
54	R8	57	ARG	3.5
43	YX	28	PHE	3.5
1	QA	1280	A	3.5
35	YP	13	ASN	3.5
13	XM	122	LYS	3.5
8	XH	94	TYR	3.5
5	QE	17	ALA	3.5
17	QQ	9	VAL	3.5
35	YP	28	GLY	3.5
54	R8	2	PRO	3.5
33	RN	119	ARG	3.5
42	RW	92	ARG	3.5
35	RP	27	HIS	3.5
25	RA	974(A)	C	3.5
54	Y8	23	VAL	3.5
33	RN	33	LEU	3.5
44	RY	2	ARG	3.5
44	YY	63	LYS	3.5
27	RD	236	GLY	3.5
8	QH	91	ARG	3.5
8	XH	91	ARG	3.5
27	RD	237	GLU	3.4
27	RD	262	ARG	3.4
30	YG	15	VAL	3.4
37	YR	69	ASP	3.4
35	YP	36	LYS	3.4
47	R1	13	ILE	3.4
27	YD	34	VAL	3.4
17	XQ	30	PRO	3.4
9	QI	15	ALA	3.4
22	XV	1	C	3.4
54	Y8	54	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
4	XD	73	ARG	3.4
17	QQ	91	ARG	3.4
20	XT	71	THR	3.4
43	RX	63	LYS	3.4
40	RU	90	VAL	3.4
38	RS	7	TYR	3.4
28	RE	79	ARG	3.4
38	RS	9	ARG	3.4
4	XD	120	LEU	3.4
1	QA	723	U	3.4
9	XI	15	ALA	3.4
4	XD	125	HIS	3.4
10	QJ	46	ARG	3.4
2	XB	188	ALA	3.3
49	R3	47	VAL	3.3
7	QG	32	ARG	3.3
17	XQ	37	LYS	3.3
38	RS	11	LYS	3.3
55	R9	13	LYS	3.3
4	QD	32	ALA	3.3
20	XT	22	ARG	3.3
39	YT	51	ARG	3.3
47	R1	95	LEU	3.3
30	YG	30	GLU	3.3
28	YE	187	ALA	3.3
43	YX	62	LYS	3.3
44	RY	21	LYS	3.3
1	QA	377	G	3.3
23	QX	3	G	3.3
4	XD	209	ARG	3.3
38	RS	8	GLU	3.3
30	RG	135	LEU	3.3
35	RP	50	ARG	3.3
55	R9	23	VAL	3.3
55	Y9	12	ASP	3.3
35	RP	13	ASN	3.3
35	RP	34	GLY	3.3
54	Y8	64	TYR	3.3
9	XI	12	GLU	3.3
10	QJ	55	LYS	3.3
36	YQ	87	LYS	3.3
9	QI	33	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
4	XD	50	ARG	3.3
9	QI	14	VAL	3.3
25	YA	887	A	3.3
43	YX	92	LEU	3.3
44	RY	23	ARG	3.3
52	R6	23	THR	3.3
17	QQ	24	GLU	3.3
33	RN	89	LYS	3.3
8	XH	2	LEU	3.2
10	XJ	43	ARG	3.2
16	XP	26	ARG	3.2
4	QD	90	GLY	3.2
4	QD	4	TYR	3.2
35	RP	81	GLN	3.2
39	YT	46	GLU	3.2
2	XB	130	ARG	3.2
12	QL	95	GLY	3.2
19	QS	2	PRO	3.2
25	YA	2179	C	3.2
1	QA	974	A	3.2
8	XH	93	VAL	3.2
33	RN	9	VAL	3.2
16	QP	31	LYS	3.2
55	Y9	30	PRO	3.2
1	QA	82	U	3.2
55	R9	14	CYS	3.2
35	YP	34	GLY	3.2
42	YW	91	GLY	3.2
16	QP	69	THR	3.2
30	YG	39	ILE	3.2
33	YN	75	TYR	3.2
27	RD	37	LEU	3.2
25	YA	1176	G	3.2
19	XS	74	PHE	3.2
29	RF	207	GLY	3.2
44	RY	103	GLY	3.2
5	QE	14	ARG	3.2
32	YI	117	GLU	3.2
33	RN	48	MET	3.2
14	XN	17	LYS	3.2
6	QF	90	VAL	3.2
13	XM	88	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
21	QU	6	ARG	3.1
27	YD	250	TRP	3.1
55	Y9	11	CYS	3.1
37	YR	38	VAL	3.1
28	YE	132	HIS	3.1
10	XJ	46	ARG	3.1
49	R3	14	GLY	3.1
4	XD	135	LEU	3.1
49	Y3	58	VAL	3.1
25	RA	2799	A	3.1
15	QO	15	PHE	3.1
12	QL	49	ASN	3.1
27	YD	111	LEU	3.1
42	YW	5	ALA	3.1
1	XA	1126	U	3.1
38	YS	13	ARG	3.1
53	R7	23	ARG	3.1
35	RP	24	GLY	3.1
1	QA	1192	C	3.1
15	XO	3	ILE	3.1
53	R7	38	GLY	3.1
1	XA	5	U	3.1
37	RR	43	GLU	3.1
42	RW	78	GLU	3.1
27	RD	258	LYS	3.1
50	Y4	68	ARG	3.1
25	RA	1070	A	3.1
8	QH	133	LEU	3.1
12	QL	93	LEU	3.1
16	QP	29	ASP	3.1
37	RR	4	LEU	3.1
20	QT	73	HIS	3.1
29	YF	154	VAL	3.0
55	Y9	5	ALA	3.0
42	RW	2	GLU	3.0
47	R1	27	GLU	3.0
1	XA	870	U	3.0
12	QL	27	LEU	3.0
15	XO	57	LEU	3.0
16	QP	60	LEU	3.0
37	YR	72	ASP	3.0
23	XX	7	G	3.0

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Mol	Chain	Res	Type	RSRZ
35	YP	82	GLY	3.0
41	YV	68	LYS	3.0
39	RT	1	MET	3.0
29	YF	96	ASP	3.0
40	YU	117	GLN	3.0
47	R1	90	ILE	3.0
2	XB	165	VAL	3.0
12	XL	96	VAL	3.0
36	RQ	104	PHE	3.0
8	QH	92	ARG	3.0
29	YF	156	LEU	3.0
41	RV	83	ARG	3.0
27	RD	26	LYS	3.0
30	RG	75	LYS	3.0
31	RH	131	VAL	3.0
25	RA	1100	C	3.0
36	RQ	20	ALA	3.0
41	RV	71	LEU	3.0
51	Y5	2	ALA	3.0
54	R8	50	LEU	3.0
3	QC	161	GLU	3.0
25	YA	2122	U	3.0
3	QC	124	ILE	3.0
27	RD	39	LYS	3.0
47	Y1	7	ILE	3.0
48	Y2	15	LYS	3.0
35	RP	91	PHE	3.0
4	XD	148	VAL	3.0
27	RD	33	LEU	3.0
4	XD	3	ARG	3.0
4	XD	76	ARG	3.0
9	XI	111	ARG	3.0
20	QT	9	ASN	3.0
34	RO	9	GLU	3.0
9	XI	7	THR	3.0
44	RY	42	VAL	3.0
27	RD	263	ARG	3.0
38	YS	3	ARG	3.0
34	YO	11	ALA	3.0
42	RW	22	ASP	3.0
20	XT	26	ASN	2.9
20	XT	74	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
21	QU	13	ILE	2.9
36	RQ	91	GLU	2.9
54	R8	65	GLU	2.9
16	XP	1	MET	2.9
15	QO	68	ARG	2.9
16	QP	18	ARG	2.9
25	RA	1058	G	2.9
1	XA	817	C	2.9
2	QB	214	ILE	2.9
27	RD	233	HIS	2.9
31	RH	148	ILE	2.9
28	RE	163	GLU	2.9
33	YN	88	GLU	2.9
2	QB	152	PHE	2.9
12	XL	10	LEU	2.9
15	QO	57	LEU	2.9
39	YT	61	PHE	2.9
28	YE	149	ARG	2.9
29	YF	173	VAL	2.9
38	RS	20	ARG	2.9
14	QN	2	ALA	2.9
7	QG	35	LYS	2.9
15	QO	3	ILE	2.9
4	XD	102	ASP	2.9
12	QL	98	TYR	2.9
49	Y3	57	GLU	2.9
16	QP	8	ARG	2.9
28	RE	99	GLY	2.9
47	Y1	21	ARG	2.9
50	R4	68	ARG	2.9
10	QJ	100	THR	2.9
31	RH	85	LYS	2.9
32	RI	118	LYS	2.9
25	RA	1078	U	2.9
40	RU	97	ASP	2.9
35	YP	65	ARG	2.9
38	YS	20	ARG	2.9
27	RD	41	GLY	2.9
27	RD	252	TRP	2.9
40	YU	19	LYS	2.9
9	XI	43	ALA	2.9
46	Y0	2	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
6	XF	84	ASN	2.9
9	QI	110	GLU	2.9
44	RY	92	ASN	2.9
1	QA	973	G	2.9
25	RA	2319	G	2.9
33	YN	53	VAL	2.9
37	YR	71	GLN	2.9
44	RY	4	LYS	2.9
4	QD	135	LEU	2.9
13	QM	96	LEU	2.9
44	YY	99	CYS	2.9
35	YP	74	GLU	2.9
17	QQ	21	VAL	2.8
21	XU	16	GLY	2.8
5	XE	129	ILE	2.8
12	QL	44	THR	2.8
38	YS	37	ALA	2.8
27	YD	15	PHE	2.8
54	Y8	48	PHE	2.8
37	YR	103	ARG	2.8
27	RD	35	LYS	2.8
31	YH	71	LEU	2.8
31	YH	75	ALA	2.8
33	RN	47	ALA	2.8
25	RA	1536	A	2.8
35	YP	15	ARG	2.8
44	YY	33	LYS	2.8
51	R5	3	LYS	2.8
55	Y9	35	ARG	2.8
11	QK	95	ILE	2.8
20	QT	70	SER	2.8
19	QS	69	HIS	2.8
30	RG	65	GLY	2.8
41	RV	77	ALA	2.8
1	XA	732	C	2.8
10	QJ	54	PHE	2.8
25	YA	1630(A)	C	2.8
27	RD	15	PHE	2.8
2	XB	27	LYS	2.8
12	XL	86	ARG	2.8
4	QD	158	ILE	2.8
27	YD	36	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
34	YO	25	LEU	2.8
43	RX	7	VAL	2.8
10	QJ	10	GLY	2.8
14	QN	13	THR	2.8
25	RA	1095	A	2.8
33	YN	90	MET	2.8
36	YQ	83	MET	2.8
13	QM	104	ARG	2.8
1	QA	1196	U	2.8
30	YG	34	LEU	2.8
33	RN	138	LEU	2.8
12	QL	48	PRO	2.8
13	QM	60	VAL	2.8
25	YA	790	C	2.8
51	R5	45	VAL	2.8
4	QD	98	GLU	2.8
6	QF	84	ASN	2.8
29	YF	47	GLY	2.8
30	RG	35	GLU	2.8
55	R9	34	GLN	2.8
44	RY	34	LYS	2.8
44	YY	21	LYS	2.8
12	QL	70	ILE	2.8
34	RO	22	ILE	2.8
40	RU	80	ILE	2.8
25	YA	529	A	2.8
41	RV	80	GLN	2.8
9	XI	11	LYS	2.8
55	Y9	2	LYS	2.8
9	QI	117	HIS	2.7
21	QU	22	ARG	2.7
30	RG	72	ARG	2.7
37	YR	2	ARG	2.7
41	RV	70	ILE	2.7
1	QA	526	C	2.7
1	QA	934	C	2.7
1	XA	1325	C	2.7
25	RA	34	C	2.7
52	Y6	13	CYS	2.7
2	XB	136	VAL	2.7
8	QH	93	VAL	2.7
15	XO	2	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
31	YH	45	VAL	2.7
10	QJ	57	LYS	2.7
47	Y1	92	LYS	2.7
19	XS	82	GLY	2.7
34	YO	74	GLY	2.7
29	YF	167	ALA	2.7
12	XL	67	THR	2.7
13	QM	103	THR	2.7
54	Y8	46	ARG	2.7
2	XB	214	ILE	2.7
1	QA	788	U	2.7
41	RV	72	VAL	2.7
44	RY	47	LYS	2.7
44	RY	102	CYS	2.7
30	RG	80	PHE	2.7
4	XD	167	GLY	2.7
9	QI	114	TYR	2.7
4	QD	120	LEU	2.7
8	QH	28	ALA	2.7
1	XA	312	C	2.7
13	QM	94	ARG	2.7
25	RA	2179	C	2.7
40	RU	2	PRO	2.7
1	QA	1190	G	2.7
25	RA	2116	G	2.7
25	RA	2125	G	2.7
25	YA	1536	A	2.7
5	QE	22	GLY	2.7
9	QI	36	TYR	2.7
11	QK	15	ALA	2.7
55	Y9	24	TYR	2.7
5	QE	83	GLU	2.7
30	RG	33	ARG	2.7
39	YT	115	ARG	2.7
1	QA	1126	U	2.7
1	QA	1450	U	2.7
40	RU	5	LYS	2.7
41	RV	76	LYS	2.7
44	RY	5	MET	2.7
51	Y5	45	VAL	2.7
31	RH	170	ARG	2.7
39	RT	97	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
55	R9	9	ARG	2.7
2	QB	108	ILE	2.7
3	XC	35	GLU	2.7
31	RH	167	GLU	2.7
54	Y8	6	THR	2.7
6	XF	54	LYS	2.7
35	RP	25	SER	2.7
35	YP	35	HIS	2.7
1	QA	5	U	2.7
1	XA	1187	G	2.7
25	YA	2121	G	2.7
37	RR	29	LEU	2.7
8	QH	85	ARG	2.7
17	XQ	101	ARG	2.7
21	XU	7	ARG	2.7
33	RN	50	ASP	2.7
36	YQ	45	GLN	2.7
38	RS	3	ARG	2.7
32	YI	109	ILE	2.7
11	QK	25	TYR	2.7
34	RO	74	GLY	2.7
5	XE	83	GLU	2.7
27	RD	181	GLU	2.7
36	YQ	112	GLU	2.7
30	YG	75	LYS	2.7
35	YP	1	MET	2.7
1	XA	135	C	2.7
1	XA	1322	C	2.7
9	QI	40	LEU	2.7
29	RF	50	SER	2.7
4	QD	178	VAL	2.6
54	R8	23	VAL	2.6
10	QJ	6	ILE	2.6
15	QO	2	PRO	2.6
43	RX	65	ARG	2.6
21	QU	14	TRP	2.6
55	Y9	36	GLN	2.6
43	YX	67	GLY	2.6
17	QQ	37	LYS	2.6
21	QU	17	THR	2.6
48	R2	31	GLU	2.6
36	YQ	104	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
12	QL	5	PRO	2.6
44	YY	66	PRO	2.6
27	YD	38	LYS	2.6
28	RE	154	LYS	2.6
40	RU	16	LYS	2.6
25	RA	2108	C	2.6
30	YG	93	THR	2.6
8	XH	136	GLU	2.6
30	RG	133	LEU	2.6
29	RF	133	ASN	2.6
8	XH	95	VAL	2.6
44	YY	72	VAL	2.6
1	XA	532	A	2.6
4	QD	114	ARG	2.6
47	Y1	11	ARG	2.6
48	R2	36	ARG	2.6
28	RE	64	LYS	2.6
33	YN	84	LYS	2.6
55	Y9	37	GLY	2.6
16	QP	68	ASP	2.6
45	YZ	44	PHE	2.6
25	RA	1374	G	2.6
25	RA	1764	G	2.6
48	Y2	34	GLU	2.6
28	RE	21	VAL	2.6
31	RH	151	ILE	2.6
39	YT	74	ARG	2.6
54	Y8	57	ARG	2.6
5	QE	49	PRO	2.6
28	RE	159	HIS	2.6
32	RI	32	PRO	2.6
20	QT	69	GLY	2.6
46	R0	76	GLY	2.6
3	QC	193	TYR	2.6
21	XU	14	TRP	2.6
1	XA	134	A	2.6
7	QG	120	ILE	2.6
11	QK	48	ILE	2.6
25	RA	1094	U	2.6
30	RG	132	ASN	2.6
4	QD	73	ARG	2.6
8	XH	18	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
11	QK	120	ARG	2.6
43	YX	60	ARG	2.6
9	XI	112	LYS	2.6
17	XQ	41	LYS	2.6
28	RE	123	ALA	2.6
55	R9	20	HIS	2.6
55	R9	32	HIS	2.6
1	QA	1517	G	2.6
8	QH	3	THR	2.6
17	XQ	42	TYR	2.6
4	QD	139	ARG	2.6
25	RA	2586	C	2.6
27	RD	227	ASN	2.6
30	YG	84	LYS	2.6
43	RX	33	LYS	2.6
44	RY	3	VAL	2.6
47	Y1	32	LYS	2.6
51	R5	57	VAL	2.6
53	Y7	47	ARG	2.6
18	XR	31	LEU	2.6
13	XM	97	PRO	2.6
54	R8	53	PRO	2.6
31	RH	123	PHE	2.6
16	XP	69	THR	2.5
27	RD	259	THR	2.5
14	QN	61	TRP	2.5
8	QH	88	LYS	2.5
12	QL	127	GLU	2.5
20	XT	8	ARG	2.5
27	RD	30	GLU	2.5
1	QA	1310	G	2.5
54	Y8	55	ALA	2.5
36	YQ	24	GLY	2.5
25	YA	2178	C	2.5
55	Y9	33	LYS	2.5
2	XB	30	ARG	2.5
8	QH	104	ARG	2.5
25	YA	2176	A	2.5
28	RE	54	GLN	2.5
29	RF	61	GLY	2.5
33	YN	36	GLY	2.5
16	QP	3	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
29	YF	48	THR	2.5
35	YP	61	ARG	2.5
47	R1	17	SER	2.5
4	QD	80	GLU	2.5
4	QD	155	LEU	2.5
39	RT	11	GLU	2.5
42	YW	23	LEU	2.5
47	Y1	97	LEU	2.5
25	RA	1099	G	2.5
25	RA	2382	G	2.5
1	QA	1140	C	2.5
25	RA	1092	C	2.5
12	XL	48	PRO	2.5
19	XS	76	PRO	2.5
31	RH	166	GLY	2.5
36	RQ	66	ILE	2.5
54	Y8	16	ILE	2.5
55	Y9	31	LYS	2.5
3	XC	164	ARG	2.5
17	QQ	101	ARG	2.5
29	YF	44	ARG	2.5
29	YF	175	THR	2.5
41	RV	82	ARG	2.5
35	RP	42	SER	2.5
12	QL	90	VAL	2.5
34	YO	24	VAL	2.5
27	RD	169	GLU	2.5
30	YG	164	GLU	2.5
3	XC	3	ASN	2.5
16	XP	29	ASP	2.5
16	XP	65	GLN	2.5
33	RN	104	LYS	2.5
39	YT	130	ALA	2.5
53	R7	48	LYS	2.5
36	YQ	122	GLY	2.5
7	XG	6	ARG	2.5
8	XH	24	THR	2.5
17	QQ	22	LEU	2.5
42	YW	92	ARG	2.5
45	RZ	91	LEU	2.5
8	QH	87	SER	2.5
4	QD	198	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
7	QG	85	TYR	2.5
27	YD	196	VAL	2.5
31	RH	157	TYR	2.5
52	R6	21	TYR	2.5
25	RA	2145	C	2.5
1	QA	506	G	2.5
1	XA	306	G	2.5
25	RA	1559	G	2.5
32	RI	10	GLU	2.5
12	XL	32	PHE	2.5
24	QY	29	U	2.5
1	QA	523	A	2.5
1	XA	389	A	2.5
20	QT	74	LYS	2.5
25	RA	1641	A	2.5
3	QC	160	ALA	2.5
3	QC	170	GLN	2.5
39	YT	97	ALA	2.5
2	XB	160	ASP	2.5
4	XD	21	LEU	2.5
12	QL	88	GLY	2.5
15	XO	34	LEU	2.5
28	RE	186	GLY	2.5
28	YE	19	ARG	2.5
30	RG	96	ARG	2.5
36	YQ	79	LEU	2.5
31	RH	155	SER	2.5
6	XF	85	VAL	2.5
31	YH	49	VAL	2.5
4	QD	125	HIS	2.4
20	QT	68	LYS	2.4
13	QM	66	LEU	2.4
30	YG	26	GLN	2.4
17	QQ	30	PRO	2.4
54	R8	46	ARG	2.4
1	QA	1194	U	2.4
1	QA	331	G	2.4
1	QA	631	G	2.4
25	YA	1630	G	2.4
27	RD	51	VAL	2.4
2	XB	152	PHE	2.4
14	QN	4	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
55	Y9	20	HIS	2.4
27	YD	37	LEU	2.4
21	QU	9	ARG	2.4
28	YE	199	ARG	2.4
44	YY	86	ARG	2.4
27	YD	238	GLY	2.4
54	R8	9	GLY	2.4
12	QL	18	VAL	2.4
12	XL	46	LYS	2.4
15	XO	60	VAL	2.4
20	XT	34	LYS	2.4
31	RH	24	VAL	2.4
31	RH	113	VAL	2.4
44	YY	79	CYS	2.4
30	RG	63	ILE	2.4
38	RS	35	ILE	2.4
3	XC	161	GLU	2.4
27	YD	237	GLU	2.4
28	RE	73	GLU	2.4
30	RG	26	GLN	2.4
33	RN	8	GLN	2.4
1	QA	1531	A	2.4
37	YR	110	PRO	2.4
55	R9	21	GLY	2.4
25	RA	2121	G	2.4
44	YY	17	SER	2.4
48	R2	15	LYS	2.4
16	QP	9	PHE	2.4
31	YH	169	VAL	2.4
53	Y7	46	VAL	2.4
7	XG	85	TYR	2.4
35	RP	106	LEU	2.4
40	YU	18	LEU	2.4
28	RE	13	ARG	2.4
35	RP	35	HIS	2.4
35	YP	27	HIS	2.4
35	YP	119	GLU	2.4
20	XT	12	ALA	2.4
37	YR	19	ALA	2.4
2	QB	91	PRO	2.4
28	RE	74	PRO	2.4
30	RG	17	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
5	QE	121	LYS	2.4
48	R2	28	LYS	2.4
49	R3	10	LYS	2.4
54	Y8	36	LYS	2.4
6	QF	72	VAL	2.4
27	RD	6	PHE	2.4
28	YE	113	PHE	2.4
24	XY	29	U	2.4
30	RG	39	ILE	2.4
20	QT	20	LEU	2.4
1	QA	1397	C	2.4
1	XA	328	C	2.4
40	YU	56	ASP	2.4
22	QV	73	A	2.4
25	YA	2799	A	2.4
16	QP	26	ARG	2.4
28	YE	111	ARG	2.4
32	YI	135	GLU	2.4
33	RN	10	GLU	2.4
35	RP	79	ARG	2.4
9	QI	119	ALA	2.4
28	YE	123	ALA	2.4
28	YE	205	ALA	2.4
37	YR	1	MET	2.4
25	RA	1063	G	2.4
25	RA	2894	G	2.4
2	QB	131	PRO	2.4
12	XL	87	GLY	2.4
28	RE	161	GLY	2.4
28	YE	106	GLY	2.4
28	YE	193	GLY	2.4
33	RN	108	PRO	2.4
3	QC	10	PHE	2.4
47	Y1	17	SER	2.4
27	RD	34	VAL	2.4
28	RE	72	VAL	2.4
20	XT	25	ARG	2.4
30	RG	97	ASP	2.4
38	YS	10	ARG	2.4
28	RE	70	ALA	2.4
28	YE	154	LYS	2.4
44	RY	88	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
4	QD	2	GLY	2.3
5	XE	22	GLY	2.3
28	RE	122	PHE	2.3
50	Y4	26	SER	2.3
51	Y5	54	GLY	2.3
1	XA	1397	C	2.3
14	XN	42	ILE	2.3
25	RA	2107	C	2.3
25	RA	2690	C	2.3
25	YA	1103	A	2.3
42	YW	86	LEU	2.3
12	XL	18	VAL	2.3
31	RH	144	VAL	2.3
52	R6	5	VAL	2.3
9	XI	66	ARG	2.3
27	RD	176	ARG	2.3
47	Y1	20	ARG	2.3
29	RF	97	TYR	2.3
1	QA	108	G	2.3
2	XB	133	LYS	2.3
19	XS	12	ASP	2.3
21	QU	26	LYS	2.3
9	XI	119	ALA	2.3
25	RA	1062	G	2.3
27	YD	184	LYS	2.3
28	YE	145	LYS	2.3
36	RQ	38	GLU	2.3
10	XJ	91	PRO	2.3
28	YE	135	HIS	2.3
32	RI	15	VAL	2.3
51	Y5	46	CYS	2.3
8	QH	84	ARG	2.3
9	XI	128	ARG	2.3
15	QO	59	MET	2.3
20	XT	17	ARG	2.3
28	RE	76	ARG	2.3
28	RE	119	ARG	2.3
9	QI	11	LYS	2.3
33	RN	7	LYS	2.3
25	RA	2117	A	2.3
49	R3	51	ALA	2.3
2	QB	146	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
4	QD	163	GLU	2.3
16	XP	34	GLU	2.3
36	YQ	38	GLU	2.3
45	YZ	97	GLU	2.3
47	Y1	27	GLU	2.3
31	YH	162	ILE	2.3
14	XN	14	PRO	2.3
19	XS	47	HIS	2.3
17	XQ	35	VAL	2.3
34	RO	58	VAL	2.3
37	YR	97	VAL	2.3
44	YY	3	VAL	2.3
13	XM	103	THR	2.3
39	RT	40	THR	2.3
10	XJ	5	ARG	2.3
13	XM	108	ARG	2.3
20	QT	25	ARG	2.3
54	R8	25	MET	2.3
25	RA	1068	G	2.3
3	QC	201	TYR	2.3
14	XN	59	ALA	2.3
39	YT	22	PHE	2.3
17	QQ	78	GLU	2.3
30	RG	137	GLU	2.3
42	YW	96	ILE	2.3
47	Y1	6	GLU	2.3
48	Y2	11	GLU	2.3
4	XD	28	SER	2.3
13	QM	6	GLY	2.3
35	YP	26	GLY	2.3
6	XF	90	VAL	2.3
27	RD	18	VAL	2.3
31	RH	43	VAL	2.3
31	YH	15	VAL	2.3
3	QC	179	ARG	2.3
4	QD	118	ARG	2.3
25	RA	1103	A	2.3
30	RG	155	MET	2.3
20	XT	13	LEU	2.3
38	RS	48	LEU	2.3
10	XJ	74	ILE	2.3
36	RQ	29	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
36	RQ	137	TYR	2.3
2	XB	170	GLU	2.3
7	XG	8	GLU	2.3
12	XL	22	SER	2.3
38	RS	52	SER	2.3
29	YF	207	GLY	2.3
50	R4	51	ASP	2.3
53	R7	46	VAL	2.3
21	XU	9	ARG	2.3
35	YP	18	ARG	2.3
47	R1	11	ARG	2.3
47	R1	26	ARG	2.3
25	YA	275	G	2.3
27	YD	33	LEU	2.3
25	YA	1060	U	2.3
3	QC	149	ALA	2.3
37	YR	14	SER	2.3
1	QA	1226	C	2.3
3	QC	130	VAL	2.3
25	RA	1064	C	2.3
47	Y1	49	VAL	2.3
54	R8	29	LYS	2.3
54	R8	49	VAL	2.3
33	RN	74	ARG	2.3
34	YO	81	ASP	2.3
36	YQ	10	ARG	2.3
30	RG	108	ASN	2.2
8	QH	2	LEU	2.2
19	QS	71	LEU	2.2
20	XT	20	LEU	2.2
29	RF	176	LEU	2.2
45	YZ	155	LEU	2.2
5	QE	21	ALA	2.2
31	RH	40	GLU	2.2
34	YO	68	GLU	2.2
48	Y2	22	GLU	2.2
4	QD	133	VAL	2.2
10	XJ	72	VAL	2.2
1	QA	1347	G	2.2
11	QK	58	PRO	2.2
27	YD	262	ARG	2.2
36	RQ	108	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
41	YV	72	VAL	2.2
53	R7	1	MET	2.2
24	QY	32	U	2.2
25	YA	669	G	2.2
26	YB	1	U	2.2
13	XM	96	LEU	2.2
37	YR	23	ASN	2.2
47	R1	66	HIS	2.2
25	RA	412	A	2.2
30	RG	29	TRP	2.2
1	QA	1322	C	2.2
3	QC	37	GLN	2.2
10	XJ	57	LYS	2.2
12	QL	28	LYS	2.2
25	RA	1765	C	2.2
31	RH	164	TYR	2.2
19	XS	81	ARG	2.2
27	RD	47	GLY	2.2
27	YD	273	ARG	2.2
37	RR	97	VAL	2.2
10	XJ	8	LEU	2.2
29	RF	81	PRO	2.2
34	YO	106	LEU	2.2
36	RQ	89	ASN	2.2
42	YW	67	ASP	2.2
54	R8	48	PHE	2.2
2	QB	140	HIS	2.2
43	YX	48	LYS	2.2
33	RN	75	TYR	2.2
42	YW	13	SER	2.2
50	R4	67	TYR	2.2
4	XD	121	VAL	2.2
9	XI	10	ARG	2.2
11	XK	126	ARG	2.2
32	RI	117	GLU	2.2
33	RN	46	VAL	2.2
43	RX	60	ARG	2.2
38	YS	60	GLY	2.2
1	QA	975	A	2.2
25	RA	276	A	2.2
25	RA	1077	A	2.2
37	YR	37	THR	2.2

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Mol	Chain	Res	Type	RSRZ
12	QL	13	LYS	2.2
12	QL	21	LYS	2.2
13	XM	120	LYS	2.2
35	RP	29	LYS	2.2
20	XT	66	ALA	2.2
4	XD	152	SER	2.2
27	RD	239	ARG	2.2
28	RE	111	ARG	2.2
29	RF	59	TYR	2.2
33	RN	107	LEU	2.2
37	YR	15	SER	2.2
4	QD	68	TYR	2.2
9	QI	125	TYR	2.2
9	QI	128	ARG	2.2
12	QL	69	TYR	2.2
33	YN	74	ARG	2.2
34	RO	17	ARG	2.2
14	QN	18	VAL	2.2
45	YZ	74	VAL	2.2
13	QM	113	PRO	2.2
31	RH	32	GLU	2.2
33	RN	105	GLY	2.2
47	Y1	87	PRO	2.2
42	YW	39	THR	2.2
20	QT	29	LYS	2.2
19	QS	12	ASP	2.2
19	QS	66	MET	2.2
27	RD	2	ALA	2.2
40	RU	46	ALA	2.2
1	QA	1451	A	2.2
1	XA	731	G	2.2
25	RA	101	G	2.2
25	RA	1093	G	2.2
27	RD	212	SER	2.2
37	YR	68	ARG	2.2
47	R1	76	ARG	2.2
49	R3	29	ARG	2.2
55	R9	18	ARG	2.2
31	RH	76	VAL	2.2
1	XA	314	C	2.2
10	XJ	4	ILE	2.2
25	RA	1694	C	2.2

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Mol	Chain	Res	Type	RSRZ
11	QK	11	LYS	2.2
33	RN	84	LYS	2.2
33	YN	1	MET	2.2
55	Y9	29	ASN	2.2
2	XB	138	LEU	2.2
10	QJ	8	LEU	2.2
19	QS	5	LEU	2.2
20	XT	24	LEU	2.2
4	QD	31	CYS	2.1
10	QJ	5	ARG	2.1
15	XO	49	ASP	2.1
25	YA	271(C)	U	2.1
27	YD	52	ARG	2.1
54	R8	34	TRP	2.1
9	XI	81	ILE	2.1
10	QJ	44	VAL	2.1
35	RP	52	GLU	2.1
36	RQ	18	LYS	2.1
14	QN	22	THR	2.1
35	YP	30	THR	2.1
1	XA	1453	G	2.1
2	QB	187	LEU	2.1
25	YA	254	G	2.1
3	XC	149	ALA	2.1
20	XT	52	ALA	2.1
38	YS	9	ARG	2.1
43	YX	65	ARG	2.1
25	RA	1886	C	2.1
25	YA	2175	C	2.1
36	YQ	12	GLN	2.1
31	YH	11	VAL	2.1
49	R3	9	VAL	2.1
10	XJ	55	LYS	2.1
17	QQ	100	LYS	2.1
17	XQ	34	LYS	2.1
31	YH	164	TYR	2.1
33	YN	7	LYS	2.1
47	Y1	69	LYS	2.1
7	XG	81	GLY	2.1
30	RG	87	PRO	2.1
30	YG	32	PRO	2.1
9	QI	64	THR	2.1

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Mol	Chain	Res	Type	RSRZ
24	QY	33	U	2.1
33	YN	67	LEU	2.1
37	YR	44	LEU	2.1
2	XB	137	ARG	2.1
7	QG	37	ASN	2.1
36	RQ	107	ALA	2.1
47	Y1	2	SER	2.1
8	QH	86	ILE	2.1
5	XE	121	LYS	2.1
31	YH	52	VAL	2.1
27	RD	200	ASP	2.1
37	YR	50	HIS	2.1
46	R0	19	LYS	2.1
25	RA	1057	A	2.1
3	XC	193	TYR	2.1
17	XQ	8	GLY	2.1
35	YP	44	GLY	2.1
4	QD	51	PRO	2.1
4	XD	97	LEU	2.1
1	QA	107	G	2.1
1	QA	576	G	2.1
1	QA	1061	G	2.1
25	YA	1093	G	2.1
25	RA	2174	C	2.1
25	YA	982	C	2.1
10	XJ	45	ARG	2.1
46	R0	74	ARG	2.1
10	XJ	50	ILE	2.1
2	QB	70	PHE	2.1
9	QI	108	VAL	2.1
15	XO	29	VAL	2.1
29	RF	139	PHE	2.1
47	Y1	4	VAL	2.1
37	YR	61	HIS	2.1
47	R1	94	LEU	2.1
54	R8	62	LEU	2.1
5	QE	122	GLU	2.1
14	XN	8	GLU	2.1
16	QP	67	THR	2.1
44	YY	2	ARG	2.1
1	QA	1183	A	2.1
25	YA	38	A	2.1

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Mol	Chain	Res	Type	RSRZ
25	YA	654(U)	A	2.1
31	YH	148	ILE	2.1
42	RW	95	ILE	2.1
12	XL	91	LYS	2.1
45	RZ	173	ALA	2.1
27	YD	12	SER	2.1
41	RV	73	SER	2.1
40	YU	94	ASN	2.1
43	RX	28	PHE	2.1
6	XF	88	VAL	2.1
1	QA	1124	G	2.1
25	YA	1059	G	2.1
25	YA	1110	G	2.1
28	RE	151	TYR	2.1
28	RE	138	PRO	2.1
33	YN	50	ASP	2.1
54	Y8	45	GLY	2.1
44	RY	32	PRO	2.1
33	YN	100	GLU	2.1
37	YR	102	GLU	2.1
39	YT	73	GLU	2.1
3	XC	30	ARG	2.1
4	QD	132	ARG	2.1
29	YF	62	ARG	2.1
1	QA	1065	U	2.1
1	XA	723	U	2.1
14	XN	15	LYS	2.1
21	XU	3	LYS	2.1
34	RO	2	ILE	2.1
47	R1	96	LYS	2.1
12	QL	68	ALA	2.1
45	YZ	172	ALA	2.1
2	QB	165	VAL	2.1
44	RY	43	ASN	2.1
6	XF	79	LEU	2.1
47	R1	74	VAL	2.1
51	R5	30	LEU	2.1
7	QG	154	TYR	2.0
8	XH	130	GLY	2.0
16	XP	30	GLY	2.0
25	RA	571	A	2.0
25	YA	276	A	2.0

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Mol	Chain	Res	Type	RSRZ
51	Y5	51	TYR	2.0
4	QD	150	GLU	2.0
5	XE	92	LYS	2.0
10	QJ	99	LYS	2.0
11	QK	124	LYS	2.0
14	XN	46	GLU	2.0
16	QP	54	GLU	2.0
33	YN	134	ARG	2.0
21	XU	13	ILE	2.0
27	RD	4	LYS	2.0
28	YE	133	LYS	2.0
37	RR	9	LYS	2.0
48	Y2	66	GLU	2.0
27	YD	272	ALA	2.0
46	R0	18	ALA	2.0
47	R1	15	ALA	2.0
29	YF	83	PHE	2.0
8	QH	95	VAL	2.0
25	YA	2111	C	2.0
26	RB	88	C	2.0
38	RS	98	VAL	2.0
1	QA	1220	G	2.0
1	XA	1181	G	2.0
25	YA	2192	G	2.0
32	RI	1	MET	2.0
22	XV	47	U	2.0
11	QK	90	GLY	2.0
27	RD	238	GLY	2.0
19	QS	80	TYR	2.0
5	XE	80	ILE	2.0
16	QP	27	LYS	2.0
17	QQ	36	ILE	2.0
19	QS	49	ILE	2.0
36	RQ	87	LYS	2.0
47	R1	7	ILE	2.0
48	Y2	67	LYS	2.0
55	R9	2	LYS	2.0
28	YE	107	THR	2.0
50	R4	44	THR	2.0
43	YX	75	ASP	2.0
28	RE	63	LEU	2.0
1	XA	1531	A	2.0

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Mol	Chain	Res	Type	RSRZ
17	QQ	5	VAL	2.0
19	QS	11	VAL	2.0
31	YH	125	VAL	2.0
32	RI	18	VAL	2.0
11	XK	118	GLY	2.0
27	RD	183	ARG	2.0
31	RH	161	GLY	2.0
28	RE	141	ILE	2.0
29	RF	171	PRO	2.0
33	RN	39	ARG	2.0
33	RN	115	ARG	2.0
36	YQ	19	GLY	2.0
38	YS	30	ARG	2.0
42	RW	4	LYS	2.0
44	RY	87	LYS	2.0
11	QK	50	TYR	2.0
11	XK	25	TYR	2.0
30	YG	17	PRO	2.0
44	YY	50	ARG	2.0
13	QM	92	HIS	2.0
5	XE	123	LEU	2.0
6	XF	22	GLU	2.0
12	XL	73	GLU	2.0
25	YA	985	C	2.0
16	XP	49	LEU	2.0
17	XQ	96	GLU	2.0
49	R3	48	GLU	2.0
1	QA	1348	U	2.0
1	XA	210	U	2.0
11	QK	89	ALA	2.0
27	RD	12	SER	2.0
8	QH	61	VAL	2.0
9	QI	65	VAL	2.0
15	QO	60	VAL	2.0
19	QS	9	VAL	2.0
45	YZ	111	VAL	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column

labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	1MG	QY	37	24/25	0.89	0.11	99,99,99,99	0
56	PPU	Z6	76	37/38	0.91	0.13	41,41,41,41	0
56	PPU	Z8	76	37/38	0.91	0.14	38,38,38,38	0
24	1MG	XY	37	24/25	0.92	0.07	59,59,59,59	0

5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3032	1/1	0.03	0.63	80,80,80,80	0
57	MG	R0	101	1/1	0.17	0.19	29,29,29,29	0
57	MG	RA	3232	1/1	0.18	0.66	80,80,80,80	0
57	MG	RA	3180	1/1	0.33	0.31	21,21,21,21	0
57	MG	RA	3065	1/1	0.34	0.63	80,80,80,80	0
57	MG	YA	3054	1/1	0.34	0.56	80,80,80,80	0
57	MG	RA	3012	1/1	0.37	0.42	7,7,7,7	0
57	MG	RP	202	1/1	0.37	0.22	65,65,65,65	0
57	MG	RA	3006	1/1	0.37	0.68	80,80,80,80	0
57	MG	RA	3216	1/1	0.37	0.30	39,39,39,39	0
57	MG	RA	3026	1/1	0.38	0.97	80,80,80,80	0
57	MG	RA	3097	1/1	0.38	0.51	80,80,80,80	0
57	MG	YA	3128	1/1	0.38	0.26	25,25,25,25	0
57	MG	RA	3222	1/1	0.39	0.20	45,45,45,45	0
57	MG	YA	3167	1/1	0.39	0.18	49,49,49,49	0
57	MG	RA	3194	1/1	0.41	0.19	54,54,54,54	0
57	MG	YA	3248	1/1	0.42	0.25	17,17,17,17	0
57	MG	YA	3208	1/1	0.43	0.20	43,43,43,43	0
57	MG	RA	3079	1/1	0.44	0.22	11,11,11,11	0
57	MG	YA	3241	1/1	0.45	0.14	34,34,34,34	0
57	MG	YA	3033	1/1	0.45	0.44	5,5,5,5	0
57	MG	YD	301	1/1	0.45	0.68	80,80,80,80	0
57	MG	YA	3025	1/1	0.47	1.18	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3018	1/1	0.47	0.44	8,8,8,8	0
57	MG	RP	201	1/1	0.47	0.52	10,10,10,10	0
57	MG	YA	3174	1/1	0.48	0.16	47,47,47,47	0
57	MG	QA	1658	1/1	0.49	0.11	90,90,90,90	0
57	MG	XA	1606	1/1	0.49	0.30	29,29,29,29	0
57	MG	RA	3138	1/1	0.50	0.15	51,51,51,51	0
57	MG	YA	3258	1/1	0.51	0.71	80,80,80,80	0
57	MG	RA	3206	1/1	0.51	0.26	40,40,40,40	0
57	MG	XA	1670	1/1	0.52	0.16	17,17,17,17	0
57	MG	YA	3153	1/1	0.52	0.17	21,21,21,21	0
57	MG	YA	3035	1/1	0.52	0.52	80,80,80,80	0
57	MG	RA	3022	1/1	0.52	0.38	1,1,1,1	0
57	MG	YA	3199	1/1	0.52	0.28	60,60,60,60	0
57	MG	YA	3109	1/1	0.53	0.78	80,80,80,80	0
57	MG	YA	3120	1/1	0.53	0.32	0,0,0,0	0
57	MG	YA	3040	1/1	0.53	0.39	0,0,0,0	0
57	MG	YA	3115	1/1	0.54	0.23	31,31,31,31	0
57	MG	YA	3103	1/1	0.56	0.44	80,80,80,80	0
57	MG	YA	3116	1/1	0.57	0.37	80,80,80,80	0
57	MG	RA	3134	1/1	0.57	0.24	24,24,24,24	0
57	MG	YA	3185	1/1	0.57	0.27	14,14,14,14	0
57	MG	YA	3002	1/1	0.58	0.95	80,80,80,80	0
57	MG	YA	3018	1/1	0.59	0.37	80,80,80,80	0
57	MG	QV	101	1/1	0.59	0.52	80,80,80,80	0
57	MG	RA	3100	1/1	0.59	0.41	36,36,36,36	0
57	MG	YA	3088	1/1	0.59	1.03	80,80,80,80	0
57	MG	RA	3163	1/1	0.60	0.35	13,13,13,13	0
57	MG	RA	3094	1/1	0.61	0.42	3,3,3,3	0
57	MG	YB	201	1/1	0.61	0.25	48,48,48,48	0
57	MG	RA	3124	1/1	0.61	0.29	35,35,35,35	0
57	MG	QA	1617	1/1	0.63	0.28	8,8,8,8	0
57	MG	RA	3082	1/1	0.64	0.33	18,18,18,18	0
57	MG	RA	3068	1/1	0.65	0.22	68,68,68,68	0
57	MG	RA	3033	1/1	0.65	0.42	5,5,5,5	0
57	MG	RA	3238	1/1	0.65	0.26	7,7,7,7	0
57	MG	YA	3175	1/1	0.66	0.16	43,43,43,43	0
57	MG	YA	3047	1/1	0.66	0.35	14,14,14,14	0
57	MG	YA	3012	1/1	0.66	0.64	80,80,80,80	0
57	MG	YA	3183	1/1	0.68	0.29	10,10,10,10	0
57	MG	YA	3043	1/1	0.68	0.27	6,6,6,6	0
57	MG	YA	3114	1/1	0.68	0.22	29,29,29,29	0
57	MG	QA	1630	1/1	0.69	0.17	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3045	1/1	0.70	0.24	20,20,20,20	0
57	MG	RA	3215	1/1	0.70	0.24	1,1,1,1	0
57	MG	YA	3161	1/1	0.70	0.06	6,6,6,6	0
57	MG	QA	1656	1/1	0.71	0.22	25,25,25,25	0
57	MG	YA	3010	1/1	0.71	0.28	0,0,0,0	0
57	MG	YA	3041	1/1	0.71	0.32	10,10,10,10	0
57	MG	R5	101	1/1	0.71	0.17	33,33,33,33	0
57	MG	YA	3223	1/1	0.71	0.19	27,27,27,27	0
57	MG	QA	1628	1/1	0.72	0.19	62,62,62,62	0
57	MG	YA	3023	1/1	0.72	0.40	6,6,6,6	0
57	MG	QA	1634	1/1	0.72	0.29	6,6,6,6	0
57	MG	YA	3089	1/1	0.72	0.35	4,4,4,4	0
57	MG	YA	3031	1/1	0.72	0.64	80,80,80,80	0
57	MG	RA	3161	1/1	0.72	0.26	75,75,75,75	0
57	MG	YA	3186	1/1	0.72	0.18	4,4,4,4	0
57	MG	YA	3187	1/1	0.72	0.13	55,55,55,55	0
57	MG	XA	1655	1/1	0.73	0.27	40,40,40,40	0
57	MG	YA	3079	1/1	0.73	0.21	22,22,22,22	0
57	MG	RA	3237	1/1	0.73	0.22	5,5,5,5	0
57	MG	YA	3049	1/1	0.73	0.33	6,6,6,6	0
57	MG	YE	301	1/1	0.73	0.27	55,55,55,55	0
57	MG	QA	1657	1/1	0.74	0.12	65,65,65,65	0
57	MG	XA	1667	1/1	0.74	0.11	32,32,32,32	0
57	MG	RA	3051	1/1	0.74	0.26	3,3,3,3	0
57	MG	YA	3160	1/1	0.74	0.24	51,51,51,51	0
57	MG	RA	3220	1/1	0.74	0.21	1,1,1,1	0
57	MG	YA	3042	1/1	0.74	0.20	2,2,2,2	0
57	MG	RA	3061	1/1	0.74	0.13	32,32,32,32	0
57	MG	YA	3050	1/1	0.75	0.47	10,10,10,10	0
57	MG	RA	3242	1/1	0.75	0.10	7,7,7,7	0
57	MG	YA	3151	1/1	0.75	0.14	26,26,26,26	0
57	MG	RA	3120	1/1	0.75	0.35	4,4,4,4	0
57	MG	QA	1603	1/1	0.75	0.22	27,27,27,27	0
57	MG	RA	3179	1/1	0.75	0.11	12,12,12,12	0
57	MG	YA	3246	1/1	0.75	0.20	7,7,7,7	0
57	MG	YA	3014	1/1	0.75	0.29	2,2,2,2	0
57	MG	YA	3256	1/1	0.75	0.28	8,8,8,8	0
57	MG	RA	3130	1/1	0.75	0.36	30,30,30,30	0
57	MG	QA	1602	1/1	0.75	0.24	9,9,9,9	0
57	MG	RA	3195	1/1	0.75	0.18	8,8,8,8	0
57	MG	RA	3088	1/1	0.75	0.28	5,5,5,5	0
57	MG	QA	1627	1/1	0.76	0.10	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3067	1/1	0.76	0.15	57,57,57,57	0
57	MG	XA	1620	1/1	0.76	0.27	5,5,5,5	0
57	MG	RA	3178	1/1	0.76	0.34	4,4,4,4	0
57	MG	RA	3156	1/1	0.76	0.27	19,19,19,19	0
57	MG	RA	3227	1/1	0.76	0.17	16,16,16,16	0
57	MG	YA	3156	1/1	0.76	0.28	6,6,6,6	0
57	MG	RA	3207	1/1	0.76	0.28	96,96,96,96	0
57	MG	YA	3006	1/1	0.76	0.34	2,2,2,2	0
57	MG	Y0	101	1/1	0.76	0.19	3,3,3,3	0
57	MG	YA	3001	1/1	0.77	0.31	0,0,0,0	0
57	MG	RA	3096	1/1	0.77	0.25	2,2,2,2	0
57	MG	YA	3110	1/1	0.77	0.32	18,18,18,18	0
57	MG	RA	3204	1/1	0.77	0.12	33,33,33,33	0
57	MG	RA	3064	1/1	0.78	0.28	12,12,12,12	0
57	MG	YA	3029	1/1	0.78	0.26	0,0,0,0	0
57	MG	QA	1637	1/1	0.78	0.18	46,46,46,46	0
57	MG	RA	3052	1/1	0.78	0.32	3,3,3,3	0
57	MG	RA	3108	1/1	0.78	0.22	3,3,3,3	0
57	MG	XA	1601	1/1	0.78	0.76	80,80,80,80	0
57	MG	RA	3034	1/1	0.78	0.28	2,2,2,2	0
57	MG	XA	1607	1/1	0.78	0.33	15,15,15,15	0
57	MG	YA	3013	1/1	0.78	0.27	1,1,1,1	0
57	MG	RA	3183	1/1	0.78	0.23	12,12,12,12	0
57	MG	YB	202	1/1	0.78	0.19	21,21,21,21	0
57	MG	YA	3184	1/1	0.78	0.20	51,51,51,51	0
57	MG	XA	1635	1/1	0.78	0.27	42,42,42,42	0
57	MG	RA	3186	1/1	0.78	0.09	71,71,71,71	0
57	MG	YA	3122	1/1	0.79	0.15	8,8,8,8	0
57	MG	QA	1638	1/1	0.79	0.17	27,27,27,27	0
57	MG	YA	3140	1/1	0.79	0.25	8,8,8,8	0
57	MG	YA	3141	1/1	0.79	0.30	7,7,7,7	0
57	MG	YA	3147	1/1	0.79	0.32	27,27,27,27	0
57	MG	RA	3212	1/1	0.79	0.25	10,10,10,10	0
57	MG	YA	3261	1/1	0.79	0.34	8,8,8,8	0
57	MG	RA	3118	1/1	0.79	0.20	13,13,13,13	0
57	MG	RA	3184	1/1	0.79	0.12	13,13,13,13	0
57	MG	YA	3095	1/1	0.79	0.32	1,1,1,1	0
57	MG	YA	3207	1/1	0.79	0.06	20,20,20,20	0
57	MG	RA	3035	1/1	0.79	0.26	1,1,1,1	0
57	MG	XA	1660	1/1	0.80	0.29	21,21,21,21	0
57	MG	XA	1661	1/1	0.80	0.16	32,32,32,32	0
57	MG	XA	1662	1/1	0.80	0.19	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3230	1/1	0.80	0.21	2,2,2,2	0
57	MG	QA	1632	1/1	0.80	0.20	25,25,25,25	0
57	MG	XA	1609	1/1	0.80	0.25	12,12,12,12	0
57	MG	YA	3032	1/1	0.80	0.37	8,8,8,8	0
57	MG	YA	3130	1/1	0.80	0.23	7,7,7,7	0
57	MG	XA	1619	1/1	0.80	0.19	13,13,13,13	0
57	MG	RA	3167	1/1	0.80	0.20	6,6,6,6	0
57	MG	RA	3174	1/1	0.80	0.25	17,17,17,17	0
57	MG	XA	1651	1/1	0.80	0.16	22,22,22,22	0
57	MG	RA	3109	1/1	0.80	0.19	26,26,26,26	0
57	MG	XA	1653	1/1	0.81	0.12	13,13,13,13	0
57	MG	RA	3046	1/1	0.81	0.30	1,1,1,1	0
57	MG	RA	3069	1/1	0.81	0.30	2,2,2,2	0
57	MG	XA	1618	1/1	0.81	0.23	26,26,26,26	0
57	MG	YA	3163	1/1	0.81	0.09	41,41,41,41	0
57	MG	RA	3071	1/1	0.81	0.23	23,23,23,23	0
57	MG	YA	3085	1/1	0.81	0.17	37,37,37,37	0
57	MG	XA	1664	1/1	0.81	0.21	8,8,8,8	0
57	MG	RA	3058	1/1	0.81	0.19	9,9,9,9	0
57	MG	RA	3240	1/1	0.81	0.22	2,2,2,2	0
57	MG	YA	3100	1/1	0.81	0.34	3,3,3,3	0
57	MG	QA	1610	1/1	0.81	0.23	3,3,3,3	0
57	MG	YA	3028	1/1	0.81	0.24	1,1,1,1	0
57	MG	YA	3152	1/1	0.81	0.29	3,3,3,3	0
57	MG	RE	302	1/1	0.82	0.22	10,10,10,10	0
57	MG	XA	1617	1/1	0.82	0.14	2,2,2,2	0
57	MG	RA	3190	1/1	0.82	0.11	8,8,8,8	0
57	MG	QA	1633	1/1	0.82	0.11	35,35,35,35	0
57	MG	RA	3153	1/1	0.82	0.16	24,24,24,24	0
57	MG	YA	3244	1/1	0.82	0.16	0,0,0,0	0
57	MG	YA	3165	1/1	0.82	0.16	7,7,7,7	0
57	MG	YA	3126	1/1	0.82	0.32	5,5,5,5	0
57	MG	YA	3172	1/1	0.82	0.16	41,41,41,41	0
57	MG	RA	3170	1/1	0.82	0.17	23,23,23,23	0
57	MG	YA	3260	1/1	0.82	0.28	2,2,2,2	0
57	MG	RA	3036	1/1	0.82	0.20	2,2,2,2	0
57	MG	YA	3044	1/1	0.82	0.13	75,75,75,75	0
57	MG	YA	3101	1/1	0.82	0.21	1,1,1,1	0
57	MG	RA	3241	1/1	0.82	0.28	29,29,29,29	0
57	MG	QA	1613	1/1	0.82	0.26	36,36,36,36	0
57	MG	YP	201	1/1	0.82	0.11	8,8,8,8	0
57	MG	YA	3009	1/1	0.82	0.27	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3024	1/1	0.83	0.18	17,17,17,17	0
57	MG	XA	1640	1/1	0.83	0.23	25,25,25,25	0
57	MG	YA	3046	1/1	0.83	0.29	0,0,0,0	0
57	MG	RA	3221	1/1	0.83	0.23	15,15,15,15	0
57	MG	RA	3092	1/1	0.83	0.24	1,1,1,1	0
57	MG	RA	3093	1/1	0.83	0.17	1,1,1,1	0
57	MG	YA	3117	1/1	0.83	0.17	11,11,11,11	0
57	MG	YA	3119	1/1	0.83	0.18	2,2,2,2	0
57	MG	RA	3055	1/1	0.83	0.30	1,1,1,1	0
57	MG	YA	3078	1/1	0.83	0.22	0,0,0,0	0
57	MG	YA	3011	1/1	0.83	0.20	2,2,2,2	0
57	MG	YA	3263	1/1	0.83	0.27	7,7,7,7	0
57	MG	RA	3013	1/1	0.83	0.25	5,5,5,5	0
57	MG	YA	3038	1/1	0.83	0.16	5,5,5,5	0
57	MG	QA	1607	1/1	0.83	0.13	5,5,5,5	0
57	MG	RA	3155	1/1	0.83	0.19	24,24,24,24	0
57	MG	XA	1623	1/1	0.83	0.23	4,4,4,4	0
57	MG	RA	3122	1/1	0.83	0.20	5,5,5,5	0
57	MG	RA	3101	1/1	0.84	0.09	32,32,32,32	0
57	MG	YA	3178	1/1	0.84	0.24	2,2,2,2	0
57	MG	RA	3201	1/1	0.84	0.17	1,1,1,1	0
57	MG	RA	3031	1/1	0.84	0.21	13,13,13,13	0
57	MG	RA	3085	1/1	0.84	0.22	4,4,4,4	0
57	MG	RA	3087	1/1	0.84	0.28	1,1,1,1	0
57	MG	YA	3017	1/1	0.84	0.29	8,8,8,8	0
57	MG	YA	3190	1/1	0.84	0.11	22,22,22,22	0
57	MG	RA	3139	1/1	0.84	0.32	12,12,12,12	0
57	MG	YA	3171	1/1	0.84	0.27	24,24,24,24	0
57	MG	RA	3053	1/1	0.84	0.23	4,4,4,4	0
57	MG	RA	3002	1/1	0.84	0.18	4,4,4,4	0
57	MG	YA	3229	1/1	0.84	0.21	30,30,30,30	0
57	MG	YA	3233	1/1	0.84	0.28	68,68,68,68	0
57	MG	YA	3239	1/1	0.84	0.22	19,19,19,19	0
57	MG	RA	3057	1/1	0.85	0.20	8,8,8,8	0
57	MG	YA	3232	1/1	0.85	0.26	5,5,5,5	0
57	MG	RA	3015	1/1	0.85	0.14	0,0,0,0	0
57	MG	YA	3237	1/1	0.85	0.19	38,38,38,38	0
57	MG	RA	3150	1/1	0.85	0.14	25,25,25,25	0
57	MG	YA	3182	1/1	0.85	0.26	30,30,30,30	0
57	MG	XA	1616	1/1	0.85	0.17	10,10,10,10	0
57	MG	QA	1660	1/1	0.85	0.18	26,26,26,26	0
57	MG	RA	3125	1/1	0.85	0.12	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3114	1/1	0.85	0.18	2,2,2,2	0
57	MG	YA	3099	1/1	0.85	0.10	2,2,2,2	0
57	MG	YA	3124	1/1	0.85	0.29	19,19,19,19	0
57	MG	RA	3217	1/1	0.85	0.18	18,18,18,18	0
57	MG	YA	3200	1/1	0.85	0.22	10,10,10,10	0
57	MG	YA	3201	1/1	0.85	0.22	2,2,2,2	0
57	MG	YA	3202	1/1	0.85	0.10	4,4,4,4	0
57	MG	YA	3205	1/1	0.85	0.16	38,38,38,38	0
57	MG	R8	101	1/1	0.85	0.16	19,19,19,19	0
57	MG	QA	1611	1/1	0.85	0.12	2,2,2,2	0
57	MG	YA	3036	1/1	0.85	0.20	7,7,7,7	0
57	MG	YA	3211	1/1	0.86	0.20	1,1,1,1	0
57	MG	YA	3221	1/1	0.86	0.16	42,42,42,42	0
57	MG	YA	3056	1/1	0.86	0.17	0,0,0,0	0
57	MG	YA	3062	1/1	0.86	0.17	5,5,5,5	0
57	MG	RA	3115	1/1	0.86	0.12	11,11,11,11	0
57	MG	RA	3117	1/1	0.86	0.10	58,58,58,58	0
57	MG	RA	3229	1/1	0.86	0.15	9,9,9,9	0
57	MG	XA	1639	1/1	0.86	0.15	13,13,13,13	0
57	MG	QA	1651	1/1	0.86	0.23	6,6,6,6	0
57	MG	YA	3131	1/1	0.86	0.15	7,7,7,7	0
57	MG	YA	3135	1/1	0.86	0.14	1,1,1,1	0
57	MG	XA	1643	1/1	0.86	0.23	34,34,34,34	0
57	MG	RA	3210	1/1	0.86	0.06	27,27,27,27	0
57	MG	XA	1602	1/1	0.86	0.29	2,2,2,2	0
57	MG	QA	1647	1/1	0.86	0.10	29,29,29,29	0
57	MG	RA	3213	1/1	0.86	0.17	42,42,42,42	0
57	MG	YA	3262	1/1	0.86	0.19	5,5,5,5	0
57	MG	XA	1608	1/1	0.86	0.21	81,81,81,81	0
57	MG	RA	3001	1/1	0.86	0.13	8,8,8,8	0
57	MG	RA	3140	1/1	0.86	0.17	17,17,17,17	0
57	MG	YA	3203	1/1	0.86	0.16	21,21,21,21	0
57	MG	RA	3143	1/1	0.86	0.27	14,14,14,14	0
57	MG	RA	3048	1/1	0.86	0.16	20,20,20,20	0
57	MG	RA	3151	1/1	0.86	0.19	10,10,10,10	0
57	MG	RA	3169	1/1	0.87	0.15	3,3,3,3	0
57	MG	YA	3197	1/1	0.87	0.20	1,1,1,1	0
57	MG	RA	3233	1/1	0.87	0.17	17,17,17,17	0
57	MG	XA	1633	1/1	0.87	0.26	33,33,33,33	0
57	MG	RA	3121	1/1	0.87	0.21	2,2,2,2	0
57	MG	RA	3224	1/1	0.87	0.11	19,19,19,19	0
57	MG	XA	1614	1/1	0.87	0.20	2,2,2,2	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3181	1/1	0.87	0.17	28,28,28,28	0
57	MG	YA	3134	1/1	0.87	0.06	11,11,11,11	0
57	MG	YA	3020	1/1	0.87	0.13	12,12,12,12	0
57	MG	YA	3021	1/1	0.87	0.26	15,15,15,15	0
57	MG	YA	3077	1/1	0.87	0.35	3,3,3,3	0
57	MG	QA	1624	1/1	0.87	0.19	49,49,49,49	0
57	MG	RA	3008	1/1	0.87	0.19	3,3,3,3	0
57	MG	YA	3082	1/1	0.87	0.22	0,0,0,0	0
57	MG	YA	3118	1/1	0.87	0.22	63,63,63,63	0
57	MG	RB	201	1/1	0.87	0.09	30,30,30,30	0
57	MG	XA	1615	1/1	0.88	0.24	2,2,2,2	0
57	MG	YA	3158	1/1	0.88	0.13	23,23,23,23	0
57	MG	RA	3066	1/1	0.88	0.21	8,8,8,8	0
57	MG	RA	3110	1/1	0.88	0.19	12,12,12,12	0
57	MG	RA	3168	1/1	0.88	0.35	55,55,55,55	0
57	MG	RA	3200	1/1	0.88	0.13	4,4,4,4	0
57	MG	RA	3113	1/1	0.88	0.10	3,3,3,3	0
57	MG	QA	1648	1/1	0.88	0.21	30,30,30,30	0
57	MG	QA	1623	1/1	0.88	0.19	41,41,41,41	0
57	MG	YA	3004	1/1	0.88	0.23	18,18,18,18	0
57	MG	YA	3005	1/1	0.88	0.15	68,68,68,68	0
57	MG	YA	3176	1/1	0.88	0.22	28,28,28,28	0
57	MG	QA	1664	1/1	0.88	0.09	24,24,24,24	0
57	MG	QA	1654	1/1	0.88	0.08	55,55,55,55	0
57	MG	YA	3127	1/1	0.88	0.15	11,11,11,11	0
57	MG	YA	3086	1/1	0.88	0.17	6,6,6,6	0
57	MG	YA	3087	1/1	0.88	0.24	8,8,8,8	0
57	MG	RA	3072	1/1	0.88	0.13	3,3,3,3	0
57	MG	XA	1642	1/1	0.88	0.20	7,7,7,7	0
57	MG	YA	3091	1/1	0.88	0.16	8,8,8,8	0
57	MG	YA	3191	1/1	0.88	0.17	23,23,23,23	0
57	MG	RA	3073	1/1	0.88	0.17	37,37,37,37	0
57	MG	YA	3096	1/1	0.88	0.20	2,2,2,2	0
57	MG	RA	3049	1/1	0.88	0.18	4,4,4,4	0
57	MG	YD	302	1/1	0.88	0.17	49,49,49,49	0
57	MG	QA	1622	1/1	0.88	0.14	44,44,44,44	0
57	MG	XA	1654	1/1	0.88	0.09	23,23,23,23	0
57	MG	QA	1625	1/1	0.88	0.08	25,25,25,25	0
57	MG	RE	301	1/1	0.89	0.17	18,18,18,18	0
57	MG	YA	3214	1/1	0.89	0.12	7,7,7,7	0
57	MG	RA	3191	1/1	0.89	0.07	26,26,26,26	0
57	MG	YA	3121	1/1	0.89	0.18	9,9,9,9	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3227	1/1	0.89	0.16	0,0,0,0	0
57	MG	RA	3193	1/1	0.89	0.06	17,17,17,17	0
57	MG	RA	3075	1/1	0.89	0.23	3,3,3,3	0
57	MG	YA	3125	1/1	0.89	0.09	10,10,10,10	0
57	MG	XA	1634	1/1	0.89	0.46	23,23,23,23	0
57	MG	RA	3076	1/1	0.89	0.20	13,13,13,13	0
57	MG	RA	3171	1/1	0.89	0.09	15,15,15,15	0
57	MG	RA	3009	1/1	0.89	0.16	84,84,84,84	0
57	MG	RA	3228	1/1	0.89	0.14	43,43,43,43	0
57	MG	RA	3203	1/1	0.89	0.12	30,30,30,30	0
57	MG	RA	3128	1/1	0.89	0.13	2,2,2,2	0
57	MG	RA	3039	1/1	0.89	0.17	2,2,2,2	0
57	MG	YA	3016	1/1	0.89	0.23	2,2,2,2	0
57	MG	YA	3143	1/1	0.89	0.08	10,10,10,10	0
57	MG	RA	3063	1/1	0.89	0.34	0,0,0,0	0
57	MG	RA	3158	1/1	0.89	0.15	12,12,12,12	0
57	MG	RA	3137	1/1	0.89	0.20	2,2,2,2	0
57	MG	QA	1605	1/1	0.89	0.26	5,5,5,5	0
57	MG	RA	3214	1/1	0.89	0.12	12,12,12,12	0
57	MG	QA	1626	1/1	0.89	0.05	10,10,10,10	0
57	MG	XA	1665	1/1	0.89	0.09	38,38,38,38	0
57	MG	YA	3073	1/1	0.89	0.20	23,23,23,23	0
57	MG	QA	1614	1/1	0.89	0.21	26,26,26,26	0
57	MG	RA	3044	1/1	0.90	0.18	2,2,2,2	0
57	MG	YA	3063	1/1	0.90	0.17	11,11,11,11	0
57	MG	YA	3070	1/1	0.90	0.14	5,5,5,5	0
57	MG	RA	3084	1/1	0.90	0.20	1,1,1,1	0
57	MG	YA	3074	1/1	0.90	0.26	0,0,0,0	0
57	MG	YA	3136	1/1	0.90	0.08	14,14,14,14	0
57	MG	QA	1604	1/1	0.90	0.18	17,17,17,17	0
57	MG	RA	3003	1/1	0.90	0.12	4,4,4,4	0
57	MG	YA	3234	1/1	0.90	0.12	1,1,1,1	0
57	MG	XA	1648	1/1	0.90	0.14	28,28,28,28	0
57	MG	RA	3234	1/1	0.90	0.16	7,7,7,7	0
57	MG	YA	3148	1/1	0.90	0.19	42,42,42,42	0
57	MG	YA	3149	1/1	0.90	0.07	17,17,17,17	0
57	MG	YA	3084	1/1	0.90	0.18	17,17,17,17	0
57	MG	RA	3235	1/1	0.90	0.13	11,11,11,11	0
57	MG	YA	3253	1/1	0.90	0.21	5,5,5,5	0
57	MG	YA	3254	1/1	0.90	0.31	1,1,1,1	0
57	MG	YA	3194	1/1	0.90	0.12	13,13,13,13	0
57	MG	YA	3257	1/1	0.90	0.25	5,5,5,5	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3196	1/1	0.90	0.26	6,6,6,6	0
57	MG	XA	1626	1/1	0.90	0.18	11,11,11,11	0
57	MG	YA	3198	1/1	0.90	0.14	16,16,16,16	0
57	MG	RA	3165	1/1	0.90	0.26	25,25,25,25	0
57	MG	YA	3052	1/1	0.90	0.11	3,3,3,3	0
57	MG	YA	3264	1/1	0.90	0.07	35,35,35,35	0
57	MG	RA	3154	1/1	0.90	0.13	17,17,17,17	0
57	MG	RA	3142	1/1	0.90	0.12	28,28,28,28	0
57	MG	YA	3058	1/1	0.90	0.25	4,4,4,4	0
57	MG	YA	3059	1/1	0.90	0.19	3,3,3,3	0
57	MG	YA	3097	1/1	0.90	0.45	11,11,11,11	0
57	MG	YA	3170	1/1	0.90	0.10	26,26,26,26	0
57	MG	YA	3209	1/1	0.90	0.09	69,69,69,69	0
57	MG	YA	3144	1/1	0.91	0.12	25,25,25,25	0
57	MG	RA	3060	1/1	0.91	0.27	65,65,65,65	0
57	MG	RA	3091	1/1	0.91	0.20	1,1,1,1	0
57	MG	YA	3092	1/1	0.91	0.16	13,13,13,13	0
57	MG	XA	1638	1/1	0.91	0.11	37,37,37,37	0
57	MG	QA	1653	1/1	0.91	0.15	16,16,16,16	0
57	MG	YA	3210	1/1	0.91	0.09	39,39,39,39	0
57	MG	RA	3062	1/1	0.91	0.47	1,1,1,1	0
57	MG	RA	3173	1/1	0.91	0.10	54,54,54,54	0
57	MG	YA	3215	1/1	0.91	0.07	25,25,25,25	0
57	MG	RA	3119	1/1	0.91	0.15	18,18,18,18	0
57	MG	YA	3222	1/1	0.91	0.13	3,3,3,3	0
57	MG	YA	3159	1/1	0.91	0.17	12,12,12,12	0
57	MG	XA	1647	1/1	0.91	0.06	44,44,44,44	0
57	MG	QA	1659	1/1	0.91	0.13	11,11,11,11	0
57	MG	YA	3162	1/1	0.91	0.16	49,49,49,49	0
57	MG	QA	1619	1/1	0.91	0.05	40,40,40,40	0
57	MG	YA	3053	1/1	0.91	0.19	1,1,1,1	0
57	MG	YA	3235	1/1	0.91	0.10	8,8,8,8	0
57	MG	YA	3236	1/1	0.91	0.19	24,24,24,24	0
57	MG	QA	1601	1/1	0.91	0.09	12,12,12,12	0
57	MG	RA	3098	1/1	0.91	0.60	80,80,80,80	0
57	MG	RA	3020	1/1	0.91	0.18	5,5,5,5	0
57	MG	YA	3242	1/1	0.91	0.10	7,7,7,7	0
57	MG	XA	1659	1/1	0.91	0.05	54,54,54,54	0
57	MG	RA	3083	1/1	0.91	0.11	12,12,12,12	0
57	MG	RA	3185	1/1	0.91	0.09	16,16,16,16	0
57	MG	YA	3250	1/1	0.91	0.17	6,6,6,6	0
57	MG	YA	3069	1/1	0.91	0.21	10,10,10,10	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3027	1/1	0.91	0.20	3,3,3,3	0
57	MG	RA	3007	1/1	0.91	0.19	26,26,26,26	0
57	MG	YA	3123	1/1	0.91	0.14	24,24,24,24	0
57	MG	QA	1665	1/1	0.91	0.12	27,27,27,27	0
57	MG	YA	3075	1/1	0.91	0.12	3,3,3,3	0
57	MG	YA	3076	1/1	0.91	0.14	2,2,2,2	0
57	MG	RA	3164	1/1	0.91	0.06	34,34,34,34	0
57	MG	RF	301	1/1	0.91	0.12	49,49,49,49	0
57	MG	XA	1669	1/1	0.91	0.10	13,13,13,13	0
57	MG	YA	3265	1/1	0.91	0.37	1,1,1,1	0
57	MG	YA	3081	1/1	0.91	0.39	0,0,0,0	0
57	MG	YA	3034	1/1	0.91	0.25	4,4,4,4	0
57	MG	RA	3086	1/1	0.91	0.15	19,19,19,19	0
57	MG	XA	1627	1/1	0.91	0.20	9,9,9,9	0
57	MG	YA	3037	1/1	0.91	0.26	7,7,7,7	0
57	MG	XA	1629	1/1	0.91	0.13	3,3,3,3	0
57	MG	QA	1640	1/1	0.91	0.08	46,46,46,46	0
58	PAR	XA	1671	42/42	0.91	0.13	40,40,40,40	0
57	MG	XA	1646	1/1	0.92	0.04	6,6,6,6	0
57	MG	RA	3104	1/1	0.92	0.14	5,5,5,5	0
57	MG	YA	3168	1/1	0.92	0.16	18,18,18,18	0
57	MG	YA	3106	1/1	0.92	0.16	84,84,84,84	0
57	MG	RA	3189	1/1	0.92	0.12	55,55,55,55	0
57	MG	YA	3204	1/1	0.92	0.12	23,23,23,23	0
57	MG	RA	3105	1/1	0.92	0.14	6,6,6,6	0
57	MG	YA	3206	1/1	0.92	0.18	25,25,25,25	0
57	MG	YA	3173	1/1	0.92	0.22	0,0,0,0	0
57	MG	RA	3209	1/1	0.92	0.07	35,35,35,35	0
57	MG	YA	3030	1/1	0.92	0.18	6,6,6,6	0
57	MG	XA	1628	1/1	0.92	0.12	28,28,28,28	0
57	MG	YA	3259	1/1	0.92	0.12	0,0,0,0	0
57	MG	YA	3177	1/1	0.92	0.14	5,5,5,5	0
57	MG	RA	3041	1/1	0.92	0.21	13,13,13,13	0
57	MG	XA	1632	1/1	0.92	0.17	36,36,36,36	0
57	MG	RD	301	1/1	0.92	0.17	11,11,11,11	0
57	MG	RA	3081	1/1	0.92	0.15	3,3,3,3	0
57	MG	RA	3029	1/1	0.92	0.20	1,1,1,1	0
57	MG	RA	3050	1/1	0.92	0.20	3,3,3,3	0
57	MG	RA	3199	1/1	0.92	0.14	60,60,60,60	0
57	MG	YA	3065	1/1	0.92	0.13	38,38,38,38	0
57	MG	RA	3025	1/1	0.92	0.11	66,66,66,66	0
57	MG	RA	3077	1/1	0.92	0.14	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3072	1/1	0.92	0.12	7,7,7,7	0
57	MG	RA	3160	1/1	0.92	0.15	10,10,10,10	0
57	MG	XX	101	1/1	0.92	0.16	11,11,11,11	0
59	ZN	QN	101	1/1	0.92	0.06	102,102,102,102	0
57	MG	XA	1668	1/1	0.93	0.09	31,31,31,31	0
57	MG	XA	1625	1/1	0.93	0.20	6,6,6,6	0
57	MG	QA	1631	1/1	0.93	0.14	15,15,15,15	0
57	MG	XA	1644	1/1	0.93	0.19	3,3,3,3	0
57	MG	RA	3004	1/1	0.93	0.37	13,13,13,13	0
57	MG	QA	1641	1/1	0.93	0.08	6,6,6,6	0
57	MG	QA	1612	1/1	0.93	0.21	5,5,5,5	0
57	MG	YA	3111	1/1	0.93	0.07	19,19,19,19	0
57	MG	XA	1630	1/1	0.93	0.06	4,4,4,4	0
57	MG	XA	1631	1/1	0.93	0.22	0,0,0,0	0
57	MG	YA	3007	1/1	0.93	0.17	4,4,4,4	0
57	MG	RA	3225	1/1	0.93	0.06	18,18,18,18	0
57	MG	RA	3239	1/1	0.93	0.13	3,3,3,3	0
57	MG	YA	3180	1/1	0.93	0.15	7,7,7,7	0
57	MG	YA	3213	1/1	0.93	0.14	17,17,17,17	0
57	MG	YA	3150	1/1	0.93	0.16	11,11,11,11	0
57	MG	RA	3040	1/1	0.93	0.13	11,11,11,11	0
57	MG	YA	3217	1/1	0.93	0.12	14,14,14,14	0
57	MG	YA	3219	1/1	0.93	0.07	17,17,17,17	0
57	MG	QA	1615	1/1	0.93	0.08	74,74,74,74	0
57	MG	XA	1637	1/1	0.93	0.06	28,28,28,28	0
57	MG	YA	3267	1/1	0.93	0.28	19,19,19,19	0
57	MG	YA	3155	1/1	0.93	0.11	38,38,38,38	0
57	MG	YA	3225	1/1	0.93	0.11	34,34,34,34	0
57	MG	YA	3226	1/1	0.93	0.17	4,4,4,4	0
57	MG	RA	3133	1/1	0.93	0.11	33,33,33,33	0
57	MG	YA	3064	1/1	0.93	0.19	4,4,4,4	0
57	MG	QA	1662	1/1	0.93	0.06	30,30,30,30	0
57	MG	YA	3067	1/1	0.93	0.30	5,5,5,5	0
57	MG	RA	3136	1/1	0.93	0.22	7,7,7,7	0
57	MG	XA	1641	1/1	0.93	0.07	2,2,2,2	0
57	MG	RA	3176	1/1	0.94	0.14	14,14,14,14	0
57	MG	RA	3177	1/1	0.94	0.14	3,3,3,3	0
57	MG	RA	3236	1/1	0.94	0.20	4,4,4,4	0
57	MG	YA	3243	1/1	0.94	0.07	0,0,0,0	0
57	MG	YA	3057	1/1	0.94	0.15	27,27,27,27	0
57	MG	YA	3245	1/1	0.94	0.23	3,3,3,3	0
57	MG	RA	3162	1/1	0.94	0.07	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	XA	1605	1/1	0.94	0.24	18,18,18,18	0
57	MG	YA	3249	1/1	0.94	0.17	3,3,3,3	0
57	MG	YA	3061	1/1	0.94	0.21	2,2,2,2	0
57	MG	YA	3251	1/1	0.94	0.28	6,6,6,6	0
57	MG	YA	3008	1/1	0.94	0.16	1,1,1,1	0
57	MG	RA	3218	1/1	0.94	0.11	4,4,4,4	0
57	MG	YA	3255	1/1	0.94	0.11	19,19,19,19	0
57	MG	RA	3219	1/1	0.94	0.12	4,4,4,4	0
57	MG	YA	3137	1/1	0.94	0.12	2,2,2,2	0
57	MG	YA	3139	1/1	0.94	0.08	19,19,19,19	0
57	MG	RA	3116	1/1	0.94	0.10	2,2,2,2	0
57	MG	RA	3123	1/1	0.94	0.16	24,24,24,24	0
57	MG	QA	1618	1/1	0.94	0.05	49,49,49,49	0
57	MG	YA	3039	1/1	0.94	0.10	0,0,0,0	0
57	MG	YA	3071	1/1	0.94	0.07	40,40,40,40	0
57	MG	RA	3019	1/1	0.94	0.16	14,14,14,14	0
57	MG	QA	1629	1/1	0.94	0.17	29,29,29,29	0
57	MG	RA	3047	1/1	0.94	0.13	1,1,1,1	0
57	MG	RA	3132	1/1	0.94	0.12	4,4,4,4	0
57	MG	YA	3019	1/1	0.94	0.24	10,10,10,10	0
57	MG	RA	3159	1/1	0.94	0.16	0,0,0,0	0
57	MG	RA	3172	1/1	0.94	0.09	4,4,4,4	0
57	MG	RA	3021	1/1	0.94	0.12	5,5,5,5	0
57	MG	XB	301	1/1	0.94	0.13	26,26,26,26	0
57	MG	RA	3145	1/1	0.94	0.11	5,5,5,5	0
58	PAR	QA	1666	42/42	0.94	0.09	58,58,58,58	0
57	MG	YA	3051	1/1	0.94	0.17	3,3,3,3	0
57	MG	XA	1645	1/1	0.94	0.21	2,2,2,2	0
57	MG	XA	1621	1/1	0.95	0.14	23,23,23,23	0
57	MG	RA	3059	1/1	0.95	0.18	4,4,4,4	0
57	MG	YA	3238	1/1	0.95	0.12	11,11,11,11	0
57	MG	YA	3080	1/1	0.95	0.17	9,9,9,9	0
57	MG	YA	3154	1/1	0.95	0.10	8,8,8,8	0
57	MG	RA	3102	1/1	0.95	0.05	4,4,4,4	0
57	MG	RA	3175	1/1	0.95	0.15	20,20,20,20	0
57	MG	YA	3157	1/1	0.95	0.28	18,18,18,18	0
57	MG	RA	3144	1/1	0.95	0.13	2,2,2,2	0
57	MG	XA	1649	1/1	0.95	0.06	33,33,33,33	0
57	MG	YA	3247	1/1	0.95	0.19	32,32,32,32	0
57	MG	QA	1639	1/1	0.95	0.12	18,18,18,18	0
57	MG	RA	3043	1/1	0.95	0.13	6,6,6,6	0
57	MG	RA	3070	1/1	0.95	0.15	6,6,6,6	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3060	1/1	0.95	0.16	3,3,3,3	0
57	MG	YA	3164	1/1	0.95	0.05	8,8,8,8	0
57	MG	RA	3166	1/1	0.95	0.12	20,20,20,20	0
57	MG	RA	3030	1/1	0.95	0.16	2,2,2,2	0
57	MG	RA	3024	1/1	0.95	0.20	28,28,28,28	0
57	MG	RA	3038	1/1	0.95	0.15	9,9,9,9	0
57	MG	YA	3132	1/1	0.95	0.05	31,31,31,31	0
57	MG	XA	1610	1/1	0.95	0.10	6,6,6,6	0
57	MG	YA	3015	1/1	0.95	0.08	4,4,4,4	0
57	MG	RA	3017	1/1	0.95	0.17	11,11,11,11	0
57	MG	RB	202	1/1	0.95	0.04	2,2,2,2	0
57	MG	YA	3218	1/1	0.95	0.10	2,2,2,2	0
57	MG	YA	3138	1/1	0.95	0.15	1,1,1,1	0
57	MG	YA	3220	1/1	0.95	0.25	2,2,2,2	0
57	MG	YA	3102	1/1	0.95	0.24	3,3,3,3	0
57	MG	XA	1666	1/1	0.95	0.05	16,16,16,16	0
57	MG	QA	1650	1/1	0.95	0.05	13,13,13,13	0
57	MG	YA	3181	1/1	0.95	0.12	4,4,4,4	0
57	MG	RA	3188	1/1	0.95	0.09	11,11,11,11	0
57	MG	RA	3211	1/1	0.95	0.07	6,6,6,6	0
57	MG	RA	3141	1/1	0.95	0.06	3,3,3,3	0
57	MG	YA	3112	1/1	0.95	0.15	11,11,11,11	0
57	MG	YA	3048	1/1	0.95	0.25	21,21,21,21	0
57	MG	RA	3231	1/1	0.95	0.27	7,7,7,7	0
57	MG	YA	3189	1/1	0.95	0.18	0,0,0,0	0
57	MG	RA	3112	1/1	0.96	0.17	5,5,5,5	0
57	MG	YA	3108	1/1	0.96	0.12	15,15,15,15	0
57	MG	RA	3135	1/1	0.96	0.07	7,7,7,7	0
57	MG	YA	3193	1/1	0.96	0.12	2,2,2,2	0
57	MG	QF	201	1/1	0.96	0.11	1,1,1,1	0
57	MG	RA	3037	1/1	0.96	0.12	15,15,15,15	0
57	MG	RA	3223	1/1	0.96	0.06	11,11,11,11	0
57	MG	RA	3192	1/1	0.96	0.14	0,0,0,0	0
57	MG	RA	3027	1/1	0.96	0.17	4,4,4,4	0
57	MG	RA	3095	1/1	0.96	0.10	2,2,2,2	0
57	MG	XA	1603	1/1	0.96	0.29	5,5,5,5	0
57	MG	QA	1645	1/1	0.96	0.12	5,5,5,5	0
57	MG	QA	1616	1/1	0.96	0.07	10,10,10,10	0
57	MG	QA	1621	1/1	0.96	0.08	7,7,7,7	0
57	MG	RA	3099	1/1	0.96	0.06	6,6,6,6	0
57	MG	YA	3252	1/1	0.96	0.27	16,16,16,16	0
57	MG	RA	3202	1/1	0.96	0.06	9,9,9,9	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3054	1/1	0.96	0.14	41,41,41,41	0
57	MG	XA	1612	1/1	0.96	0.15	7,7,7,7	0
57	MG	RA	3010	1/1	0.96	0.35	4,4,4,4	0
57	MG	RA	3148	1/1	0.96	0.24	39,39,39,39	0
57	MG	RA	3056	1/1	0.96	0.07	21,21,21,21	0
57	MG	RA	3208	1/1	0.96	0.08	29,29,29,29	0
57	MG	QA	1643	1/1	0.96	0.11	1,1,1,1	0
57	MG	RA	3045	1/1	0.96	0.12	23,23,23,23	0
57	MG	RA	3127	1/1	0.96	0.12	10,10,10,10	0
57	MG	YA	3133	1/1	0.96	0.08	8,8,8,8	0
57	MG	XA	1656	1/1	0.96	0.04	10,10,10,10	0
57	MG	YA	3055	1/1	0.96	0.23	4,4,4,4	0
57	MG	YA	3266	1/1	0.96	0.10	1,1,1,1	0
57	MG	QA	1644	1/1	0.96	0.04	34,34,34,34	0
57	MG	RA	3129	1/1	0.96	0.07	21,21,21,21	0
57	MG	XA	1624	1/1	0.96	0.04	23,23,23,23	0
57	MG	RA	3157	1/1	0.96	0.20	1,1,1,1	0
57	MG	RA	3089	1/1	0.96	0.14	2,2,2,2	0
57	MG	RA	3131	1/1	0.96	0.11	0,0,0,0	0
57	MG	YA	3142	1/1	0.96	0.11	28,28,28,28	0
57	MG	RA	3005	1/1	0.96	0.26	6,6,6,6	0
57	MG	RA	3111	1/1	0.96	0.12	1,1,1,1	0
57	MG	YA	3145	1/1	0.96	0.17	16,16,16,16	0
57	MG	YA	3146	1/1	0.96	0.12	4,4,4,4	0
57	MG	YA	3224	1/1	0.97	0.10	5,5,5,5	0
57	MG	QA	1642	1/1	0.97	0.10	20,20,20,20	0
57	MG	XA	1652	1/1	0.97	0.08	1,1,1,1	0
57	MG	RA	3016	1/1	0.97	0.08	1,1,1,1	0
57	MG	YA	3228	1/1	0.97	0.14	9,9,9,9	0
57	MG	RA	3226	1/1	0.97	0.10	26,26,26,26	0
57	MG	YA	3231	1/1	0.97	0.04	2,2,2,2	0
57	MG	XV	101	1/1	0.97	0.12	3,3,3,3	0
57	MG	YA	3179	1/1	0.97	0.05	4,4,4,4	0
57	MG	RA	3028	1/1	0.97	0.14	2,2,2,2	0
57	MG	XA	1613	1/1	0.97	0.07	0,0,0,0	0
57	MG	XA	1658	1/1	0.97	0.04	0,0,0,0	0
57	MG	YA	3094	1/1	0.97	0.04	0,0,0,0	0
57	MG	RA	3205	1/1	0.97	0.06	7,7,7,7	0
57	MG	RA	3152	1/1	0.97	0.12	3,3,3,3	0
57	MG	YA	3022	1/1	0.97	0.13	2,2,2,2	0
57	MG	YA	3098	1/1	0.97	0.08	2,2,2,2	0
57	MG	QA	1655	1/1	0.97	0.04	6,6,6,6	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3197	1/1	0.97	0.06	12,12,12,12	0
57	MG	RA	3198	1/1	0.97	0.09	7,7,7,7	0
57	MG	YA	3192	1/1	0.97	0.04	6,6,6,6	0
57	MG	QA	1608	1/1	0.97	0.04	11,11,11,11	0
57	MG	RA	3074	1/1	0.97	0.06	10,10,10,10	0
57	MG	QA	1606	1/1	0.97	0.12	5,5,5,5	0
57	MG	YA	3107	1/1	0.97	0.14	22,22,22,22	0
57	MG	YA	3129	1/1	0.97	0.15	0,0,0,0	0
57	MG	RA	3078	1/1	0.98	0.05	5,5,5,5	0
57	MG	XA	1657	1/1	0.98	0.08	27,27,27,27	0
57	MG	XA	1604	1/1	0.98	0.22	13,13,13,13	0
57	MG	RA	3187	1/1	0.98	0.07	10,10,10,10	0
57	MG	XA	1622	1/1	0.98	0.08	9,9,9,9	0
57	MG	QA	1609	1/1	0.98	0.04	9,9,9,9	0
57	MG	YA	3230	1/1	0.98	0.03	10,10,10,10	0
57	MG	QA	1620	1/1	0.98	0.03	22,22,22,22	0
57	MG	XA	1663	1/1	0.98	0.03	29,29,29,29	0
57	MG	RA	3090	1/1	0.98	0.22	3,3,3,3	0
57	MG	YA	3104	1/1	0.98	0.09	3,3,3,3	0
57	MG	YA	3105	1/1	0.98	0.12	1,1,1,1	0
57	MG	RA	3023	1/1	0.98	0.08	0,0,0,0	0
57	MG	QA	1635	1/1	0.98	0.04	8,8,8,8	0
57	MG	XA	1611	1/1	0.98	0.18	3,3,3,3	0
57	MG	QA	1646	1/1	0.98	0.06	36,36,36,36	0
57	MG	YA	3240	1/1	0.98	0.08	23,23,23,23	0
57	MG	RA	3147	1/1	0.98	0.12	0,0,0,0	0
57	MG	RA	3182	1/1	0.98	0.10	23,23,23,23	0
57	MG	RA	3196	1/1	0.98	0.24	8,8,8,8	0
57	MG	XM	201	1/1	0.98	0.08	26,26,26,26	0
57	MG	QM	201	1/1	0.98	0.05	25,25,25,25	0
57	MG	QA	1661	1/1	0.98	0.10	9,9,9,9	0
57	MG	YA	3066	1/1	0.98	0.16	6,6,6,6	0
57	MG	YA	3166	1/1	0.98	0.16	45,45,45,45	0
57	MG	RA	3107	1/1	0.98	0.03	3,3,3,3	0
57	MG	XA	1636	1/1	0.98	0.10	5,5,5,5	0
57	MG	RA	3042	1/1	0.99	0.07	14,14,14,14	0
57	MG	RA	3149	1/1	0.99	0.05	15,15,15,15	0
57	MG	QA	1663	1/1	0.99	0.04	33,33,33,33	0
57	MG	YA	3083	1/1	0.99	0.03	7,7,7,7	0
57	MG	RA	3080	1/1	0.99	0.11	2,2,2,2	0
57	MG	YA	3068	1/1	0.99	0.11	3,3,3,3	0
57	MG	QA	1649	1/1	0.99	0.04	2,2,2,2	0

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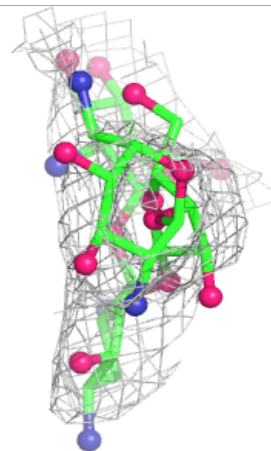
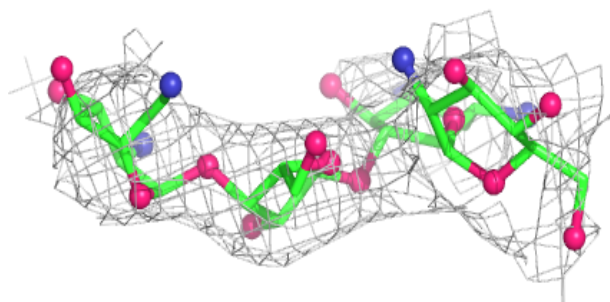
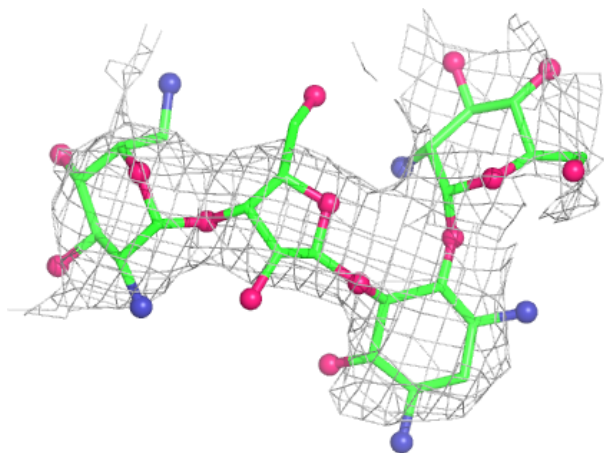
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3103	1/1	0.99	0.08	1,1,1,1	0
57	MG	YA	3188	1/1	0.99	0.04	4,4,4,4	0
57	MG	YA	3212	1/1	0.99	0.06	17,17,17,17	0
57	MG	RA	3014	1/1	0.99	0.10	2,2,2,2	0
57	MG	YA	3026	1/1	0.99	0.42	32,32,32,32	0
57	MG	YA	3169	1/1	0.99	0.02	3,3,3,3	0
57	MG	YA	3216	1/1	0.99	0.06	38,38,38,38	0
57	MG	YA	3090	1/1	0.99	0.11	14,14,14,14	0
57	MG	QA	1652	1/1	0.99	0.02	0,0,0,0	0
57	MG	RA	3106	1/1	0.99	0.10	3,3,3,3	0
57	MG	YB	203	1/1	0.99	0.08	33,33,33,33	0
57	MG	YA	3195	1/1	0.99	0.04	0,0,0,0	0
57	MG	YA	3093	1/1	0.99	0.06	8,8,8,8	0
57	MG	YA	3113	1/1	0.99	0.08	2,2,2,2	0
57	MG	QA	1636	1/1	0.99	0.03	13,13,13,13	0
57	MG	RA	3146	1/1	0.99	0.03	3,3,3,3	0
57	MG	XA	1650	1/1	0.99	0.04	27,27,27,27	0
57	MG	YA	3003	1/1	0.99	0.04	9,9,9,9	0
57	MG	RA	3126	1/1	0.99	0.03	8,8,8,8	0
59	ZN	XD	301	1/1	0.99	0.13	5,5,5,5	0
59	ZN	XN	101	1/1	0.99	0.07	82,82,82,82	0
59	ZN	QD	301	1/1	1.00	0.12	21,21,21,21	0
57	MG	RA	3011	1/1	1.00	0.09	5,5,5,5	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

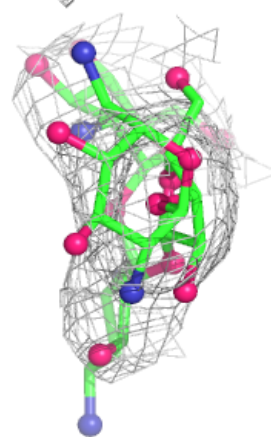
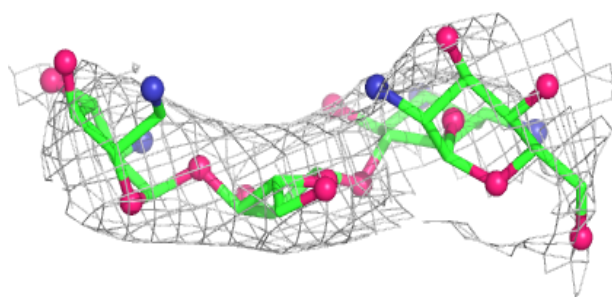
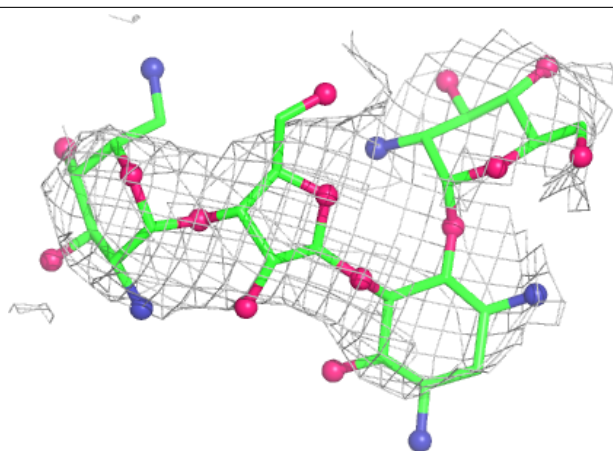
Electron density around PAR XA 1671:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PAR QA 1666:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



5.5 Other polymers [i](#)

There are no such residues in this entry.