



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 10:31 AM UTC

PDB ID : 7A18 / pdb_00007a18
Title : 50S Deinococcus radiodurans ribosome bounded with mycinamicin IV
Authors : Breiner, E.; Eyal, Z.; Matzov, D.; Halfon, Y.; Cimicata, G.; Rozenberg, H.;
Zimmerman, E.; Bashan, A.; Yonath, A.
Deposited on : 2020-08-12
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : **FAILED**
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
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

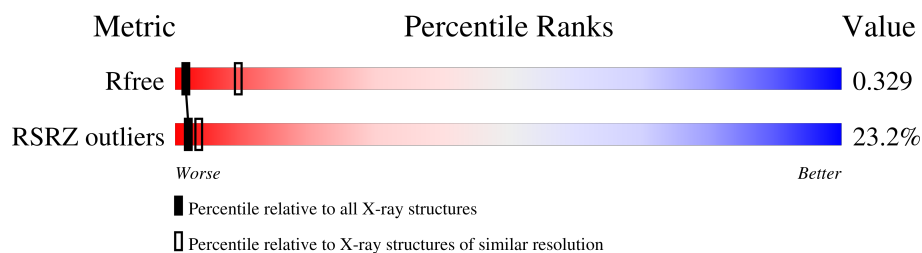
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1001 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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
30	MG	3	101	-	-	-	X
30	MG	I	201	-	-	-	X
30	MG	N	201	-	-	-	X
30	MG	Q	101	-	-	-	X
30	MG	W	101	-	-	-	X
30	MG	X	2902	-	-	-	X
30	MG	X	2903	-	-	-	X
30	MG	X	2916	-	-	-	X
30	MG	X	2918	-	-	-	X
30	MG	X	2920	-	-	-	X
30	MG	X	2925	-	-	-	X
30	MG	X	2927	-	-	-	X
30	MG	X	2931	-	-	-	X
30	MG	X	2944	-	-	-	X
30	MG	X	2945	-	-	-	X
30	MG	X	2949	-	-	-	X
30	MG	X	2957	-	-	-	X
30	MG	X	2960	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	MG	X	2961	-	-	-	X
30	MG	X	2962	-	-	-	X
30	MG	X	2963	-	-	-	X
30	MG	X	2966	-	-	-	X
30	MG	X	2969	-	-	-	X
30	MG	X	2971	-	-	-	X
30	MG	X	2976	-	-	-	X
30	MG	X	2978	-	-	-	X
30	MG	X	2979	-	-	-	X
30	MG	X	2983	-	-	-	X
30	MG	X	2988	-	-	-	X
30	MG	X	2989	-	-	-	X
30	MG	X	2996	-	-	-	X
30	MG	X	2999	-	-	-	X
30	MG	X	3002	-	-	-	X
30	MG	X	3008	-	-	-	X
30	MG	X	3010	-	-	-	X
30	MG	X	3015	-	-	-	X
30	MG	X	3016	-	-	-	X
30	MG	X	3017	-	-	-	X
30	MG	X	3036	-	-	-	X
30	MG	X	3040	-	-	-	X
30	MG	X	3044	-	-	-	X
30	MG	X	3045	-	-	-	X
30	MG	X	3047	-	-	-	X
30	MG	X	3048	-	-	-	X
30	MG	X	3051	-	-	-	X
30	MG	X	3057	-	-	-	X
30	MG	X	3060	-	-	-	X
30	MG	X	3064	-	-	-	X
30	MG	X	3065	-	-	-	X
30	MG	X	3068	-	-	-	X
30	MG	X	3071	-	-	-	X
30	MG	X	3082	-	-	-	X
30	MG	X	3093	-	-	-	X
30	MG	X	3095	-	-	-	X
30	MG	X	3097	-	-	-	X
30	MG	X	3098	-	-	-	X
30	MG	X	3104	-	-	-	X
30	MG	X	3107	-	-	-	X
30	MG	X	3109	-	-	-	X
30	MG	X	3110	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	MG	X	3115	-	-	-	X
30	MG	X	3122	-	-	-	X
30	MG	X	3124	-	-	-	X
30	MG	X	3134	-	-	-	X
30	MG	X	3136	-	-	-	X
30	MG	X	3141	-	-	-	X
30	MG	X	3143	-	-	-	X
30	MG	X	3149	-	-	-	X
30	MG	X	3153	-	-	-	X
30	MG	X	3154	-	-	-	X
30	MG	X	3156	-	-	-	X
30	MG	X	3163	-	-	-	X
30	MG	Y	201	-	-	-	X
30	MG	Y	202	-	-	-	X
30	MG	Y	203	-	-	-	X
31	SPD	X	3166	-	-	-	X
31	SPD	X	3168	-	-	-	X

2 Entry composition

There are 31 unique types of molecules in this entry. The entry contains 84387 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 RNA (2699-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	2699	Total	C	N	O	P	0	1	0
			57957	25853	10701	18704	2699			

- Molecule 2 is a RNA chain called RNA (122-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	122	Total	C	N	O	P	0	0	0
			2598	1161	476	840	121			

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	271	Total	C	N	O	S	0	0	0
			2001	1246	390	362	3			

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	206	Total	C	N	O	S	0	0	0
			1544	968	296	272	8			

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	195	Total	C	N	O	S	0	0	0
			1467	912	280	273	2			

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	176	Total	C	N	O	S	0	0	0
			1367	870	238	253	6			

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	171	Total	C	N	O	S	0	0	0
			1286	812	237	236	1			

- Molecule 8 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	G	142	Total	C	N	O	S	0	0	0
			1107	698	208	198	3			

- Molecule 9 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	134	Total	C	N	O	S	0	0	0
			993	611	197	180	5			

- Molecule 10 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	137	Total	C	N	O	S	0	0	0
			982	603	194	184	1			

- Molecule 11 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	134	Total	C	N	O	S	0	0	0
			1042	668	188	179	7			

- Molecule 12 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	115	Total	C	N	O	S	0	0	0
			897	552	183	159	3			

- Molecule 13 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	L	104	Total	C	N	O	0	0	0
			751	457	154	140			

- Molecule 14 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	M	118	Total	C	N	O			
			923	578	178	167	0	0	0

- Molecule 15 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	N	117	Total	C	N	O	S		
			962	599	203	159	1	0	0

- Molecule 16 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
16	O	98	Total	C	N	O	S		
			734	459	135	139	1	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	12	ALA	TYR	conflict	UNP Q9RY64

- Molecule 17 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	P	129	Total	C	N	O	S		
			1020	643	199	176	2	0	0

- Molecule 18 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	Q	93	Total	C	N	O	S		
			718	452	134	130	2	0	0

- Molecule 19 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	R	110	Total	C	N	O	S		
			793	492	149	151	1	0	0

- Molecule 20 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	S	175	Total	C	N	O	S	0	0	1
			1290	811	224	251	4			

- Molecule 21 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	T	72	Total	C	N	O	S	0	0	0
			542	343	104	94	1			

- Molecule 22 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	U	74	Total	C	N	O		0	0	0
			539	336	107	96				

- Molecule 23 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	V	54	Total	C	N	O	S	0	0	0
			438	270	89	78	1			

- Molecule 24 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	W	55	Total	C	N	O	S	0	0	0
			424	264	82	76	2			

- Molecule 25 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Z	57	Total	C	N	O	S	0	0	0
			448	275	92	76	5			

- Molecule 26 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	1	49	Total	C	N	O		0	0	0
			315	199	54	62				

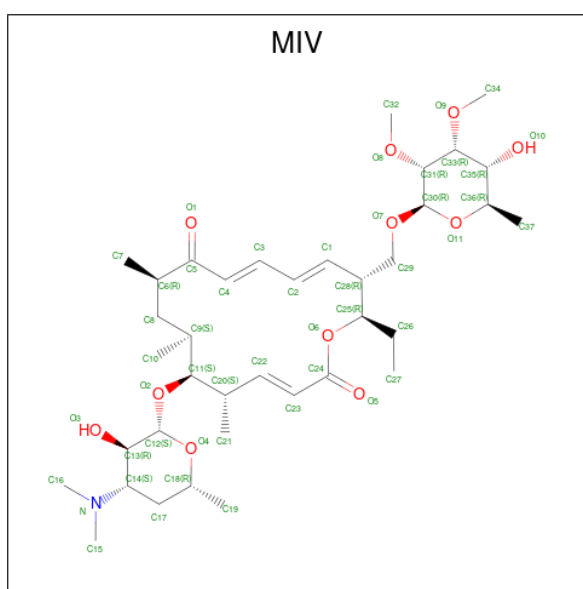
- Molecule 27 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	2	46	Total	C	N	O	S	0	0	0
			383	230	91	60	2			

- Molecule 28 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	3	63	Total	C	N	O	S	0	0	0
			470	295	97	75	3			

- Molecule 29 is MYCINAMICIN IV (CCD ID: MIV) (formula: $C_{37}H_{61}NO_{11}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	X	1	Total	C	N	O	0	0
			49	37	1	11		

- Molecule 30 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

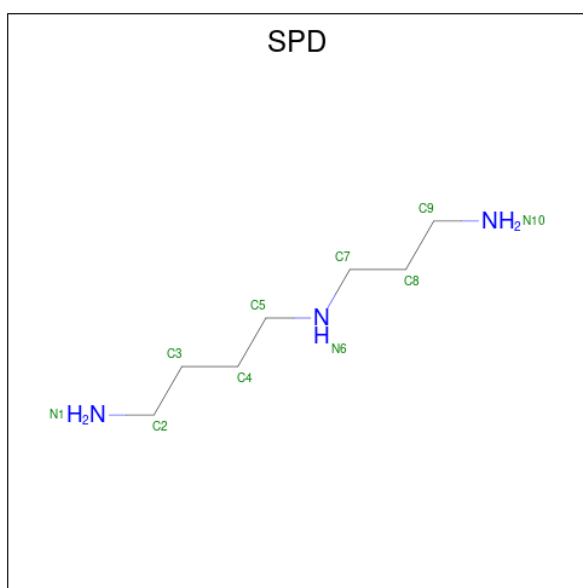
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	X	264	Total	Mg	0	0
			264	264		
30	Y	4	Total	Mg	0	0
			4	4		
30	A	1	Total	Mg	0	0
			1	1		
30	I	1	Total	Mg	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	N	1	Total	Mg	0	0
			1	1		
30	Q	2	Total	Mg	0	0
			2	2		
30	W	1	Total	Mg	0	0
			1	1		
30	2	2	Total	Mg	0	0
			2	2		
30	3	1	Total	Mg	0	0
			1	1		

- Molecule 31 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	X	1	Total	C	N	0	0
			10	7	3		
31	X	1	Total	C	N	0	0
			10	7	3		
31	X	1	Total	C	N	0	0
			10	7	3		
31	X	1	Total	C	N	0	0
			10	7	3		
31	X	1	Total	C	N	0	0
			10	7	3		
31	X	1	Total	C	N	0	0
			10	7	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	V	1	Total	C	N	0	0
			10	7	3		

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

3 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	169.59Å 410.13Å 690.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.40 50.00 – 3.40	Depositor EDS
% Data completeness (in resolution range)	93.9 (50.00-3.40) 94.0 (50.00-3.40)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.284 , 0.318 0.295 , 0.329	Depositor DCC
R_{free} test set	16405 reflections (4.58%)	wwPDB-VP
Wilson B-factor (Å ²)	79.6	Xtriage
Anisotropy	0.724	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 100.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	84387	wwPDB-VP
Average B, all atoms (Å ²)	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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

4.2 Too-close contacts [i](#)

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

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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

4.3.2 Protein sidechains [i](#)

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

4.3.3 RNA [i](#)

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

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

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 285 ligands modelled in this entry, 277 are monoatomic - leaving 8 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
31	SPD	X	3167	1	9,9,9	0.32	0	8,8,8	1.00	0
31	SPD	X	3170	1	9,9,9	0.46	0	8,8,8	1.21	1 (12%)
31	SPD	X	3171	-	9,9,9	0.28	0	8,8,8	0.66	0
29	MIV	X	2901	-	51,51,51	0.73	2 (3%)	64,71,71	1.52	8 (12%)
31	SPD	X	3168	1	9,9,9	0.41	0	8,8,8	0.97	0
31	SPD	X	3166	-	9,9,9	0.37	0	8,8,8	0.64	0
31	SPD	X	3169	1	9,9,9	0.37	0	8,8,8	1.08	1 (12%)
31	SPD	V	101	-	9,9,9	0.29	0	8,8,8	0.86	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	SPD	X	3167	1	-	2/7/7/7	-
31	SPD	X	3170	1	-	4/7/7/7	-
31	SPD	X	3171	-	-	3/7/7/7	-
29	MIV	X	2901	-	-	26/55/91/91	0/2/3/3
31	SPD	X	3168	1	-	2/7/7/7	-
31	SPD	X	3166	-	-	3/7/7/7	-
31	SPD	X	3169	1	-	3/7/7/7	-
31	SPD	V	101	-	-	5/7/7/7	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	X	2901	MIV	C31-C33	2.83	1.58	1.52
29	X	2901	MIV	O6-C24	2.83	1.40	1.34

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	2901	MIV	O6-C25-C26	-5.97	97.39	106.90
29	X	2901	MIV	C6-C8-C9	4.49	123.14	115.09
29	X	2901	MIV	O6-C25-C28	4.19	116.68	107.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	2901	MIV	C32-O8-C31	3.96	124.64	114.47
29	X	2901	MIV	O11-C30-C31	3.63	116.55	109.49

There are no chirality outliers.

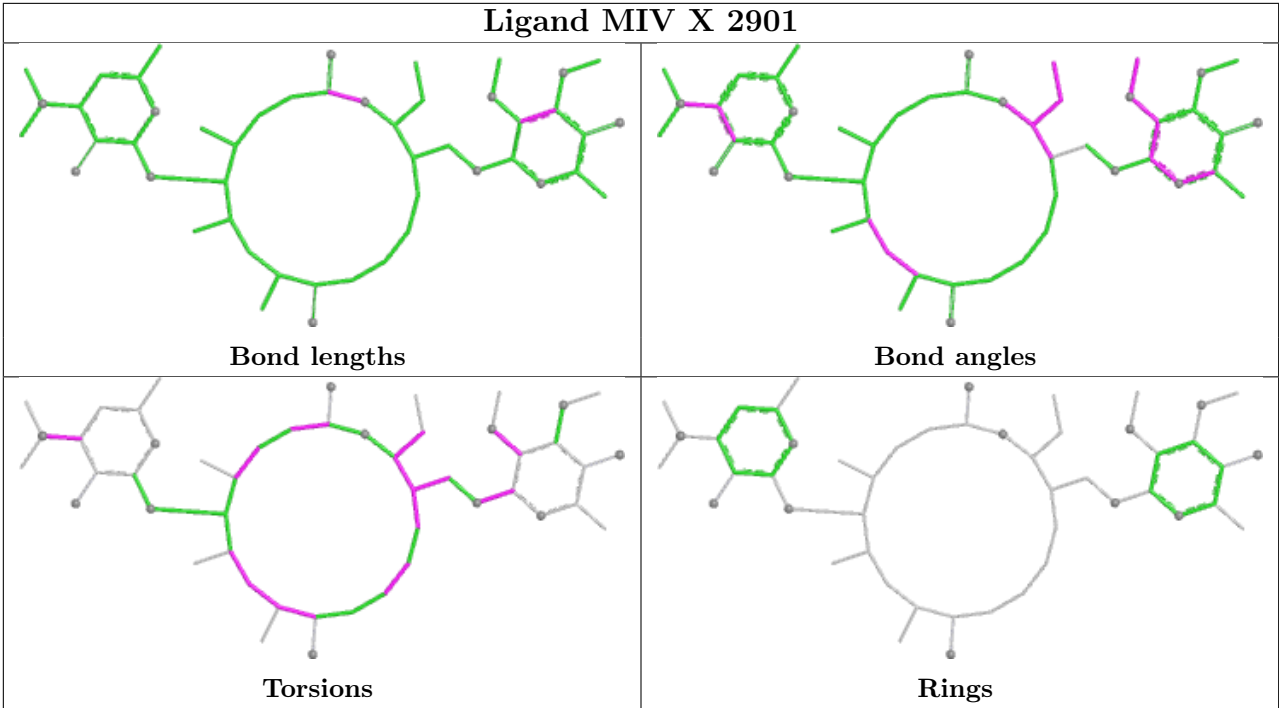
5 of 48 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	X	2901	MIV	C17-C14-N-C15
29	X	2901	MIV	C13-C14-N-C15
29	X	2901	MIV	C5-C6-C8-C9
29	X	2901	MIV	O1-C5-C6-C7
29	X	2901	MIV	C4-C5-C6-C7

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	X	12

The worst 5 of 12 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	X	282:A	O3'	302:U	P	65.10
1	X	362:C	O3'	380:C	P	54.16
1	X	2090:U	O3'	2165:A	P	19.14
1	X	1184:G	O3'	1191:G	P	18.52
1	X	2773:G	O3'	2779:A	P	17.92

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	X	2699/2699 (100%)	1.06	394 (14%) 6 7	37, 96, 191, 312	1 (0%)
2	Y	122/122 (100%)	1.31	23 (18%) 3 4	95, 183, 226, 251	0
3	A	271/271 (100%)	2.35	129 (47%) 0 1	79, 131, 162, 170	0
4	B	206/206 (100%)	1.18	34 (16%) 4 6	40, 64, 80, 85	0
5	C	195/195 (100%)	1.50	51 (26%) 1 3	60, 122, 150, 159	0
6	D	176/176 (100%)	2.10	77 (43%) 0 1	168, 207, 227, 235	0
7	E	171/171 (100%)	1.66	55 (32%) 1 1	98, 144, 186, 190	0
8	G	142/142 (100%)	1.54	43 (30%) 1 2	60, 95, 107, 115	0
9	H	134/134 (100%)	1.02	19 (14%) 6 8	46, 57, 64, 69	0
10	I	137/137 (100%)	2.38	56 (40%) 0 1	67, 141, 180, 192	0
11	J	134/134 (100%)	1.72	47 (35%) 1 1	71, 103, 126, 132	0
12	K	115/115 (100%)	0.89	12 (10%) 11 12	40, 47, 54, 58	0
13	L	104/104 (100%)	2.59	54 (51%) 0 0	159, 198, 226, 237	0
14	M	118/118 (100%)	0.80	12 (10%) 12 12	46, 56, 69, 74	0
15	N	117/117 (100%)	1.73	41 (35%) 1 1	59, 94, 121, 127	0
16	O	98/98 (100%)	1.30	19 (19%) 3 4	66, 114, 134, 138	0
17	P	129/129 (100%)	0.97	21 (16%) 4 6	49, 59, 82, 97	0
18	Q	93/93 (100%)	1.58	22 (23%) 2 3	85, 109, 125, 126	0
19	R	110/110 (100%)	1.60	32 (29%) 1 2	86, 103, 146, 156	0
20	S	175/175 (100%)	1.72	48 (27%) 1 2	113, 157, 176, 182	0
21	T	72/72 (100%)	1.76	22 (30%) 1 2	87, 133, 147, 153	0
22	U	74/74 (100%)	2.84	47 (63%) 0 0	106, 144, 175, 178	0
23	V	54/54 (100%)	1.56	16 (29%) 1 2	116, 127, 154, 162	0
24	W	55/55 (100%)	1.10	9 (16%) 4 6	88, 108, 128, 133	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Z	57/57 (100%)	1.09	7 (12%) 8 9	47, 56, 70, 74	0
26	1	49/49 (100%)	2.50	26 (53%) 0 0	132, 148, 166, 168	0
27	2	46/46 (100%)	1.79	19 (41%) 0 1	63, 86, 94, 96	0
28	3	63/63 (100%)	2.68	40 (63%) 0 0	105, 115, 128, 134	0
All	All	5916/5916 (100%)	1.39	1375 (23%) 2 3	37, 105, 203, 312	1 (0%)

The worst 5 of 1375 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	S	82	ASP	13.1
20	S	67	LYS	10.6
10	I	48	PHE	10.5
10	I	67	ASN	10.5
13	L	12	ARG	10.4

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

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

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(Å ²)	Q<0.9
30	MG	3	101	1/1	0.18	0.99	126,126,126,126	0
30	MG	X	2976	1/1	0.28	0.98	125,125,125,125	0
30	MG	Q	101	1/1	0.29	0.54	104,104,104,104	0
30	MG	X	3154	1/1	0.36	0.93	74,74,74,74	0
30	MG	X	3098	1/1	0.39	1.25	120,120,120,120	0
30	MG	X	3017	1/1	0.42	0.95	114,114,114,114	0
30	MG	X	3097	1/1	0.43	0.51	102,102,102,102	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	SPD	X	3166	10/10	0.43	0.65	92,95,99,99	0
30	MG	X	3141	1/1	0.44	0.70	145,145,145,145	0
30	MG	X	3104	1/1	0.45	0.58	119,119,119,119	0
30	MG	X	2902	1/1	0.45	0.57	82,82,82,82	0
30	MG	X	3032	1/1	0.47	0.37	112,112,112,112	0
30	MG	X	2918	1/1	0.47	0.78	71,71,71,71	0
30	MG	Y	202	1/1	0.47	0.48	98,98,98,98	0
30	MG	X	3082	1/1	0.48	0.48	112,112,112,112	0
30	MG	X	3040	1/1	0.50	0.68	103,103,103,103	0
30	MG	X	3109	1/1	0.50	0.43	63,63,63,63	0
30	MG	X	3093	1/1	0.52	0.52	117,117,117,117	0
30	MG	X	2971	1/1	0.52	0.49	59,59,59,59	0
30	MG	Y	204	1/1	0.52	0.32	151,151,151,151	0
30	MG	X	3077	1/1	0.53	0.40	56,56,56,56	0
30	MG	X	3048	1/1	0.53	0.47	124,124,124,124	0
30	MG	X	3143	1/1	0.55	0.45	133,133,133,133	0
30	MG	X	2978	1/1	0.55	0.58	85,85,85,85	0
30	MG	I	201	1/1	0.55	0.98	81,81,81,81	0
30	MG	X	2903	1/1	0.56	0.48	60,60,60,60	0
30	MG	X	2962	1/1	0.57	0.43	97,97,97,97	0
30	MG	X	3163	1/1	0.58	0.88	60,60,60,60	0
30	MG	X	3050	1/1	0.60	0.34	108,108,108,108	0
30	MG	X	2977	1/1	0.60	0.36	66,66,66,66	0
30	MG	X	2945	1/1	0.61	0.68	104,104,104,104	0
30	MG	X	3015	1/1	0.62	0.52	105,105,105,105	0
30	MG	X	3139	1/1	0.62	0.34	182,182,182,182	0
30	MG	X	2960	1/1	0.62	0.45	62,62,62,62	0
30	MG	X	3120	1/1	0.63	0.36	78,78,78,78	0
30	MG	X	2989	1/1	0.63	0.45	103,103,103,103	0
30	MG	X	3051	1/1	0.63	0.43	118,118,118,118	0
30	MG	X	2963	1/1	0.63	0.42	96,96,96,96	0
30	MG	X	3044	1/1	0.64	0.60	73,73,73,73	0
30	MG	X	3149	1/1	0.65	0.44	83,83,83,83	0
30	MG	X	2944	1/1	0.65	0.59	102,102,102,102	0
30	MG	X	3102	1/1	0.65	0.15	112,112,112,112	0
30	MG	X	3146	1/1	0.66	0.21	178,178,178,178	0
30	MG	X	3065	1/1	0.66	1.16	99,99,99,99	0
30	MG	X	2936	1/1	0.66	0.24	69,69,69,69	0
30	MG	X	2990	1/1	0.66	0.30	62,62,62,62	0
30	MG	X	3115	1/1	0.66	0.51	54,54,54,54	0
30	MG	X	2957	1/1	0.67	0.77	73,73,73,73	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MG	X	2979	1/1	0.67	0.87	83,83,83,83	0
30	MG	X	3134	1/1	0.67	0.41	39,39,39,39	0
30	MG	X	3056	1/1	0.67	0.22	47,47,47,47	0
30	MG	X	3057	1/1	0.68	0.41	80,80,80,80	0
30	MG	X	3008	1/1	0.68	0.53	49,49,49,49	0
30	MG	X	3071	1/1	0.68	0.40	95,95,95,95	0
30	MG	X	3072	1/1	0.68	0.27	115,115,115,115	0
30	MG	X	2940	1/1	0.69	0.30	60,60,60,60	0
30	MG	X	2949	1/1	0.70	0.67	56,56,56,56	0
30	MG	X	3064	1/1	0.70	0.58	113,113,113,113	0
30	MG	X	3016	1/1	0.70	0.69	72,72,72,72	0
30	MG	X	3126	1/1	0.70	0.38	76,76,76,76	0
30	MG	X	3036	1/1	0.70	0.82	75,75,75,75	0
30	MG	X	3107	1/1	0.70	1.16	83,83,83,83	0
30	MG	X	3158	1/1	0.71	0.35	64,64,64,64	0
30	MG	X	2965	1/1	0.71	0.25	117,117,117,117	0
30	MG	X	3055	1/1	0.71	0.39	66,66,66,66	0
30	MG	X	3039	1/1	0.71	0.23	67,67,67,67	0
31	SPD	X	3170	10/10	0.71	0.31	62,63,64,64	0
31	SPD	X	3168	10/10	0.72	0.43	44,45,46,46	0
30	MG	X	2983	1/1	0.72	0.40	89,89,89,89	0
30	MG	Y	203	1/1	0.73	0.43	132,132,132,132	0
30	MG	X	3026	1/1	0.73	0.36	81,81,81,81	0
30	MG	X	3151	1/1	0.73	0.39	53,53,53,53	0
30	MG	X	2920	1/1	0.73	0.51	74,74,74,74	0
30	MG	X	2927	1/1	0.73	0.53	69,69,69,69	0
30	MG	X	3159	1/1	0.73	0.28	93,93,93,93	0
30	MG	X	3121	1/1	0.73	0.14	79,79,79,79	0
31	SPD	X	3169	10/10	0.73	0.26	77,79,80,81	0
30	MG	X	3060	1/1	0.73	0.57	54,54,54,54	0
30	MG	X	3074	1/1	0.74	0.24	59,59,59,59	0
30	MG	X	3046	1/1	0.75	0.31	78,78,78,78	0
30	MG	W	101	1/1	0.75	0.52	111,111,111,111	0
30	MG	X	3095	1/1	0.75	0.46	65,65,65,65	0
30	MG	X	3010	1/1	0.75	0.96	111,111,111,111	0
30	MG	X	3002	1/1	0.75	0.66	138,138,138,138	0
30	MG	X	3130	1/1	0.75	0.29	60,60,60,60	0
30	MG	N	201	1/1	0.75	0.51	75,75,75,75	0
30	MG	X	3047	1/1	0.76	0.41	92,92,92,92	0
30	MG	X	2966	1/1	0.76	0.48	101,101,101,101	0
30	MG	X	3140	1/1	0.76	0.36	159,159,159,159	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MG	X	3122	1/1	0.76	0.66	65,65,65,65	0
30	MG	X	3045	1/1	0.76	0.43	92,92,92,92	0
30	MG	X	2950	1/1	0.76	0.34	88,88,88,88	0
30	MG	X	3144	1/1	0.77	0.37	105,105,105,105	0
30	MG	X	3037	1/1	0.77	0.32	104,104,104,104	0
30	MG	X	2988	1/1	0.77	0.60	87,87,87,87	0
30	MG	X	2916	1/1	0.77	0.70	62,62,62,62	0
30	MG	X	3131	1/1	0.77	0.32	98,98,98,98	0
30	MG	X	3058	1/1	0.77	0.32	63,63,63,63	0
30	MG	X	2941	1/1	0.77	0.31	73,73,73,73	0
30	MG	X	3061	1/1	0.77	0.40	95,95,95,95	0
30	MG	X	2984	1/1	0.77	0.26	62,62,62,62	0
30	MG	X	3052	1/1	0.77	0.16	105,105,105,105	0
30	MG	X	2910	1/1	0.78	0.22	41,41,41,41	0
30	MG	X	3136	1/1	0.78	0.45	79,79,79,79	0
30	MG	Y	201	1/1	0.78	0.40	114,114,114,114	0
30	MG	X	3091	1/1	0.78	0.37	53,53,53,53	0
30	MG	X	3110	1/1	0.78	0.41	41,41,41,41	0
31	SPD	X	3167	10/10	0.78	0.33	56,56,57,57	0
30	MG	X	3068	1/1	0.78	0.47	97,97,97,97	0
30	MG	A	301	1/1	0.78	0.38	94,94,94,94	0
30	MG	X	2931	1/1	0.78	0.46	68,68,68,68	0
30	MG	X	3070	1/1	0.79	0.09	136,136,136,136	0
30	MG	X	2969	1/1	0.79	0.48	55,55,55,55	0
30	MG	X	2914	1/1	0.79	0.36	65,65,65,65	0
30	MG	X	2961	1/1	0.79	0.58	78,78,78,78	0
30	MG	X	2925	1/1	0.79	0.41	50,50,50,50	0
30	MG	X	3123	1/1	0.79	0.24	85,85,85,85	0
30	MG	X	3153	1/1	0.79	0.44	47,47,47,47	0
30	MG	X	3124	1/1	0.79	0.55	67,67,67,67	0
30	MG	X	3156	1/1	0.79	0.42	71,71,71,71	0
30	MG	X	3111	1/1	0.80	0.30	53,53,53,53	0
30	MG	X	3014	1/1	0.80	0.41	75,75,75,75	0
30	MG	X	3164	1/1	0.80	0.36	39,39,39,39	0
30	MG	X	3085	1/1	0.80	0.33	75,75,75,75	0
30	MG	X	3086	1/1	0.80	0.62	78,78,78,78	0
30	MG	X	2912	1/1	0.80	0.75	64,64,64,64	0
30	MG	X	2996	1/1	0.80	0.85	76,76,76,76	0
30	MG	X	2999	1/1	0.80	0.56	81,81,81,81	0
30	MG	X	3096	1/1	0.80	0.69	71,71,71,71	0
31	SPD	V	101	10/10	0.80	0.29	126,128,135,136	0
30	MG	X	3090	1/1	0.81	0.32	81,81,81,81	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MG	X	3105	1/1	0.81	0.41	69,69,69,69	0
30	MG	X	2906	1/1	0.81	0.31	75,75,75,75	0
30	MG	X	3084	1/1	0.81	0.40	82,82,82,82	0
30	MG	X	3087	1/1	0.81	0.29	116,116,116,116	0
30	MG	X	3162	1/1	0.81	0.50	69,69,69,69	0
30	MG	X	2921	1/1	0.82	0.47	66,66,66,66	0
30	MG	X	3009	1/1	0.82	0.24	54,54,54,54	0
30	MG	X	2958	1/1	0.82	0.63	77,77,77,77	0
30	MG	X	3083	1/1	0.82	0.82	79,79,79,79	0
30	MG	X	3147	1/1	0.82	0.38	95,95,95,95	0
30	MG	X	3073	1/1	0.82	0.36	118,118,118,118	0
30	MG	2	101	1/1	0.82	0.49	80,80,80,80	0
30	MG	X	3080	1/1	0.83	0.25	51,51,51,51	0
30	MG	X	2934	1/1	0.83	0.23	58,58,58,58	0
30	MG	X	3067	1/1	0.83	0.18	94,94,94,94	0
30	MG	X	3019	1/1	0.83	0.24	91,91,91,91	0
30	MG	X	2908	1/1	0.83	0.54	39,39,39,39	0
30	MG	X	3030	1/1	0.83	0.32	48,48,48,48	0
30	MG	X	2905	1/1	0.83	0.33	62,62,62,62	0
30	MG	X	2928	1/1	0.83	0.33	68,68,68,68	0
30	MG	X	3127	1/1	0.83	0.15	49,49,49,49	0
30	MG	X	3128	1/1	0.83	0.39	95,95,95,95	0
30	MG	X	2930	1/1	0.83	0.31	50,50,50,50	0
30	MG	X	2923	1/1	0.83	0.28	75,75,75,75	0
30	MG	X	2959	1/1	0.84	0.48	78,78,78,78	0
30	MG	X	3101	1/1	0.84	0.60	95,95,95,95	0
30	MG	X	2917	1/1	0.84	0.42	71,71,71,71	0
29	MIV	X	2901	49/49	0.84	0.22	52,53,57,58	0
30	MG	X	3076	1/1	0.84	0.30	65,65,65,65	0
30	MG	X	3062	1/1	0.84	0.45	109,109,109,109	0
30	MG	X	2985	1/1	0.84	0.31	63,63,63,63	0
30	MG	X	3092	1/1	0.85	0.52	77,77,77,77	0
30	MG	X	3118	1/1	0.85	0.19	45,45,45,45	0
30	MG	X	2951	1/1	0.85	0.41	54,54,54,54	0
30	MG	X	2913	1/1	0.85	0.34	59,59,59,59	0
30	MG	X	2964	1/1	0.85	0.32	67,67,67,67	0
30	MG	X	2975	1/1	0.85	0.23	84,84,84,84	0
30	MG	X	3018	1/1	0.85	0.43	76,76,76,76	0
30	MG	X	2948	1/1	0.85	0.35	83,83,83,83	0
30	MG	X	3103	1/1	0.86	0.17	61,61,61,61	0
30	MG	X	3161	1/1	0.86	0.38	38,38,38,38	0
30	MG	X	3145	1/1	0.86	0.20	77,77,77,77	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MG	X	2937	1/1	0.86	1.22	83,83,83,83	0
30	MG	X	3034	1/1	0.86	0.23	66,66,66,66	0
30	MG	X	2955	1/1	0.86	0.57	68,68,68,68	0
30	MG	X	2956	1/1	0.86	0.32	69,69,69,69	0
30	MG	X	2929	1/1	0.86	0.25	71,71,71,71	0
30	MG	X	3125	1/1	0.86	0.38	71,71,71,71	0
30	MG	X	3028	1/1	0.86	0.76	69,69,69,69	0
30	MG	X	2980	1/1	0.86	0.46	88,88,88,88	0
30	MG	X	2909	1/1	0.87	0.27	44,44,44,44	0
30	MG	X	2952	1/1	0.87	0.40	52,52,52,52	0
30	MG	2	102	1/1	0.87	0.23	62,62,62,62	0
30	MG	X	3088	1/1	0.87	0.25	78,78,78,78	0
30	MG	X	3000	1/1	0.87	0.31	67,67,67,67	0
30	MG	X	3023	1/1	0.87	0.94	70,70,70,70	0
30	MG	X	2972	1/1	0.87	0.45	81,81,81,81	0
30	MG	X	2992	1/1	0.87	0.51	73,73,73,73	0
30	MG	X	3094	1/1	0.87	0.89	69,69,69,69	0
30	MG	X	3066	1/1	0.87	0.28	81,81,81,81	0
30	MG	X	3054	1/1	0.88	0.28	101,101,101,101	0
30	MG	X	3112	1/1	0.88	0.48	54,54,54,54	0
30	MG	X	3033	1/1	0.88	0.15	45,45,45,45	0
30	MG	X	3116	1/1	0.88	0.12	60,60,60,60	0
30	MG	X	3117	1/1	0.88	0.34	48,48,48,48	0
30	MG	X	3025	1/1	0.88	0.65	38,38,38,38	0
30	MG	X	3119	1/1	0.88	0.26	69,69,69,69	0
30	MG	X	3160	1/1	0.88	0.54	40,40,40,40	0
30	MG	X	3035	1/1	0.88	0.30	104,104,104,104	0
30	MG	X	2973	1/1	0.88	0.30	69,69,69,69	0
30	MG	X	2987	1/1	0.88	0.24	54,54,54,54	0
30	MG	X	2954	1/1	0.88	0.44	56,56,56,56	0
30	MG	X	3108	1/1	0.88	0.36	61,61,61,61	0
30	MG	X	2947	1/1	0.88	0.13	87,87,87,87	0
30	MG	X	3043	1/1	0.88	0.11	47,47,47,47	0
30	MG	X	3129	1/1	0.89	0.13	86,86,86,86	0
30	MG	X	3150	1/1	0.89	0.25	70,70,70,70	0
30	MG	X	3049	1/1	0.89	0.42	124,124,124,124	0
30	MG	Q	102	1/1	0.89	0.16	75,75,75,75	0
30	MG	X	2911	1/1	0.89	0.63	39,39,39,39	0
30	MG	X	2981	1/1	0.89	0.38	79,79,79,79	0
31	SPD	X	3171	10/10	0.89	0.35	45,47,50,50	0
30	MG	X	3142	1/1	0.89	0.14	83,83,83,83	0
30	MG	X	3041	1/1	0.90	0.18	114,114,114,114	0

Continued on next page...

Continued from previous page...

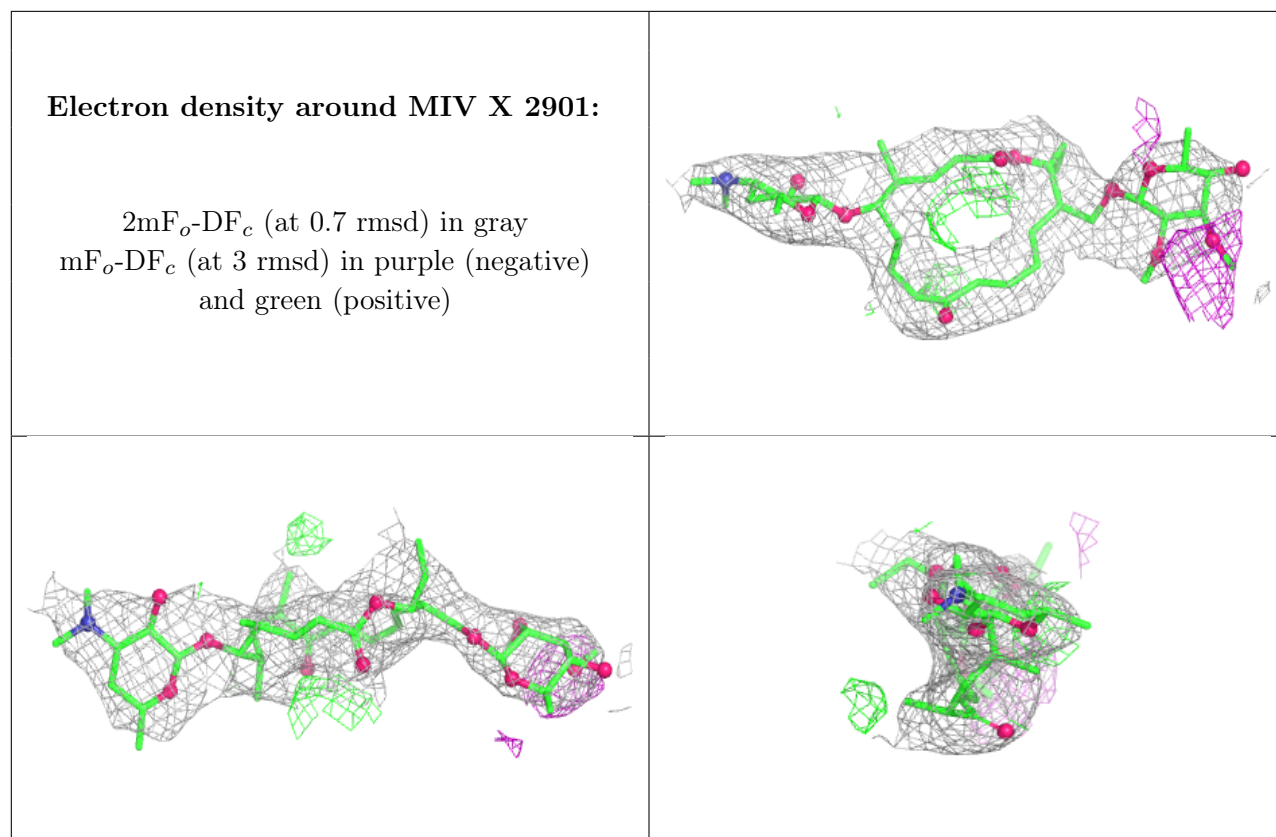
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MG	X	2991	1/1	0.90	0.10	80,80,80,80	0
30	MG	X	2982	1/1	0.90	0.17	101,101,101,101	0
30	MG	X	3089	1/1	0.90	0.40	61,61,61,61	0
30	MG	X	3069	1/1	0.90	0.24	90,90,90,90	0
30	MG	X	3133	1/1	0.90	0.09	50,50,50,50	0
30	MG	X	2935	1/1	0.90	0.17	90,90,90,90	0
30	MG	X	2970	1/1	0.90	0.23	61,61,61,61	0
30	MG	X	3011	1/1	0.90	0.33	53,53,53,53	0
30	MG	X	2904	1/1	0.90	0.24	49,49,49,49	0
30	MG	X	3135	1/1	0.91	0.26	148,148,148,148	0
30	MG	X	3063	1/1	0.91	0.16	112,112,112,112	0
30	MG	X	3024	1/1	0.91	0.08	41,41,41,41	0
30	MG	X	2924	1/1	0.91	0.34	80,80,80,80	0
30	MG	X	3042	1/1	0.91	0.16	58,58,58,58	0
30	MG	X	2942	1/1	0.91	0.29	49,49,49,49	0
30	MG	X	3003	1/1	0.91	0.45	77,77,77,77	0
30	MG	X	3004	1/1	0.91	0.58	61,61,61,61	0
30	MG	X	2943	1/1	0.91	0.42	67,67,67,67	0
30	MG	X	3099	1/1	0.91	0.07	69,69,69,69	0
30	MG	X	3100	1/1	0.91	0.09	77,77,77,77	0
30	MG	X	2946	1/1	0.92	0.33	51,51,51,51	0
30	MG	X	3132	1/1	0.92	0.20	88,88,88,88	0
30	MG	X	3007	1/1	0.92	0.20	71,71,71,71	0
30	MG	X	3021	1/1	0.92	0.47	73,73,73,73	0
30	MG	X	3113	1/1	0.92	0.36	55,55,55,55	0
30	MG	X	3079	1/1	0.92	0.13	55,55,55,55	0
30	MG	X	3029	1/1	0.93	0.22	66,66,66,66	0
30	MG	X	2922	1/1	0.93	0.52	51,51,51,51	0
30	MG	X	2974	1/1	0.93	0.26	61,61,61,61	0
30	MG	X	3075	1/1	0.93	0.25	72,72,72,72	0
30	MG	X	3148	1/1	0.93	0.09	72,72,72,72	0
30	MG	X	2953	1/1	0.93	0.49	57,57,57,57	0
30	MG	X	3013	1/1	0.93	0.14	62,62,62,62	0
30	MG	X	2939	1/1	0.93	0.20	50,50,50,50	0
30	MG	X	2993	1/1	0.93	0.32	128,128,128,128	0
30	MG	X	2968	1/1	0.93	0.26	75,75,75,75	0
30	MG	X	3155	1/1	0.93	0.12	54,54,54,54	0
30	MG	X	3038	1/1	0.93	0.47	67,67,67,67	0
30	MG	X	2998	1/1	0.93	0.18	78,78,78,78	0
30	MG	X	2994	1/1	0.94	0.30	88,88,88,88	0
30	MG	X	3114	1/1	0.94	0.30	48,48,48,48	0
30	MG	X	3001	1/1	0.94	0.06	91,91,91,91	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MG	X	3138	1/1	0.94	0.15	39,39,39,39	0
30	MG	X	2915	1/1	0.94	0.43	57,57,57,57	0
30	MG	X	2986	1/1	0.94	0.15	57,57,57,57	0
30	MG	X	2907	1/1	0.94	0.33	46,46,46,46	0
30	MG	X	3005	1/1	0.94	0.10	101,101,101,101	0
30	MG	X	3059	1/1	0.95	0.20	55,55,55,55	0
30	MG	X	3053	1/1	0.95	0.22	53,53,53,53	0
30	MG	X	3012	1/1	0.95	0.09	47,47,47,47	0
30	MG	X	3078	1/1	0.95	0.11	59,59,59,59	0
30	MG	X	3152	1/1	0.95	0.19	49,49,49,49	0
30	MG	X	3022	1/1	0.95	0.09	64,64,64,64	0
30	MG	X	3165	1/1	0.96	0.42	39,39,39,39	0
30	MG	X	3006	1/1	0.96	0.23	44,44,44,44	0
30	MG	X	3027	1/1	0.96	0.21	50,50,50,50	0
30	MG	X	2932	1/1	0.96	0.13	49,49,49,49	0
30	MG	X	3106	1/1	0.96	0.06	64,64,64,64	0
30	MG	X	3020	1/1	0.96	0.11	88,88,88,88	0
30	MG	X	2997	1/1	0.96	0.23	99,99,99,99	0
30	MG	X	2933	1/1	0.97	0.13	61,61,61,61	0
30	MG	X	2967	1/1	0.97	0.11	86,86,86,86	0
30	MG	X	3137	1/1	0.97	0.09	83,83,83,83	0
30	MG	X	3081	1/1	0.97	0.09	76,76,76,76	0
30	MG	X	2919	1/1	0.97	0.50	44,44,44,44	0
30	MG	X	2926	1/1	0.98	0.18	55,55,55,55	0
30	MG	X	2938	1/1	0.98	0.14	52,52,52,52	0
30	MG	X	3031	1/1	0.98	0.16	38,38,38,38	0
30	MG	X	2995	1/1	0.98	0.11	54,54,54,54	0
30	MG	X	3157	1/1	0.99	0.11	45,45,45,45	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.



5.5 Other polymers [i](#)

There are no such residues in this entry.