



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:35 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 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

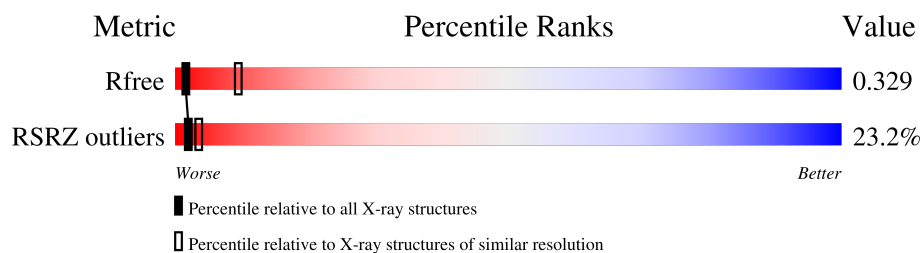
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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

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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

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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				

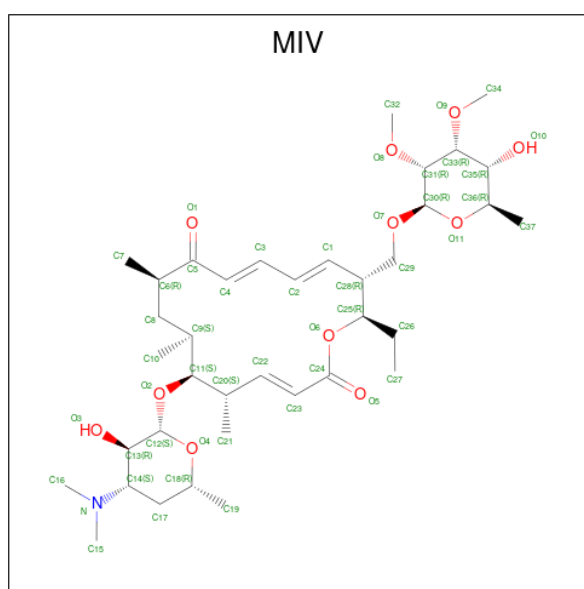
- Molecule 27 is a protein called 50S ribosomal protein L34.

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).

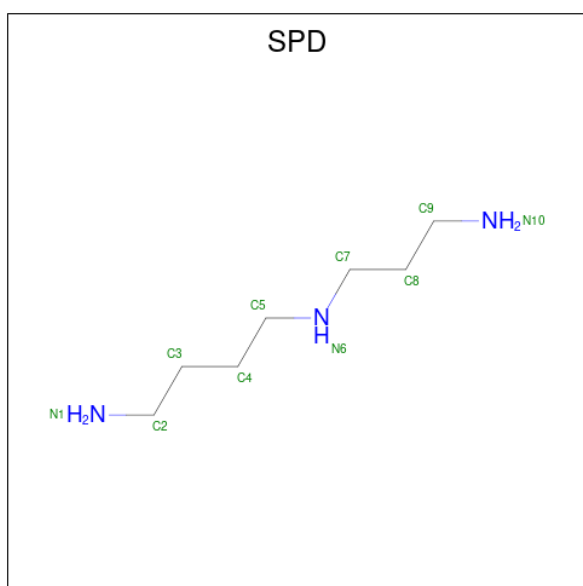
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	X	264	Total	Mg	0	0
			264	264		
30	Y	4	Total	Mg	0	0
			4	4		
30	A	1	Total	Mg	0	0
			1	1		
30	I	1	Total	Mg	0	0
			1	1		

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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		

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

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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](#)

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4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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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

All (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

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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
31	X	3170	SPD	C8-C7-N6	2.91	119.88	112.07
29	X	2901	MIV	C30-O11-C36	2.27	117.50	113.63
31	X	3169	SPD	C7-N6-C5	2.16	123.65	113.40
29	X	2901	MIV	C27-C26-C25	-2.09	107.69	113.23
29	X	2901	MIV	C13-C14-N	2.00	116.71	110.94

There are no chirality outliers.

All (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
29	X	2901	MIV	C2-C1-C28-C29
29	X	2901	MIV	O6-C25-C28-C1
29	X	2901	MIV	C26-C25-C28-C1
29	X	2901	MIV	C26-C25-C28-C29
29	X	2901	MIV	C1-C28-C29-O7
29	X	2901	MIV	C25-C28-C29-O7
29	X	2901	MIV	O11-C30-O7-C29
29	X	2901	MIV	C30-C31-O8-C32
31	X	3170	SPD	C4-C5-N6-C7
31	X	3171	SPD	C4-C5-N6-C7
31	V	101	SPD	C3-C4-C5-N6
29	X	2901	MIV	C17-C14-N-C16
31	X	3168	SPD	C2-C3-C4-C5
31	X	3169	SPD	C3-C4-C5-N6
29	X	2901	MIV	C11-C20-C22-C23
29	X	2901	MIV	C31-C30-O7-C29
31	X	3169	SPD	C2-C3-C4-C5
29	X	2901	MIV	C1-C2-C3-C4
29	X	2901	MIV	C22-C23-C24-O6
29	X	2901	MIV	C21-C20-C22-C23
31	X	3166	SPD	C2-C3-C4-C5
31	X	3170	SPD	C2-C3-C4-C5
31	X	3169	SPD	C7-C8-C9-N10
31	V	101	SPD	C7-C8-C9-N10
29	X	2901	MIV	C7-C6-C8-C9

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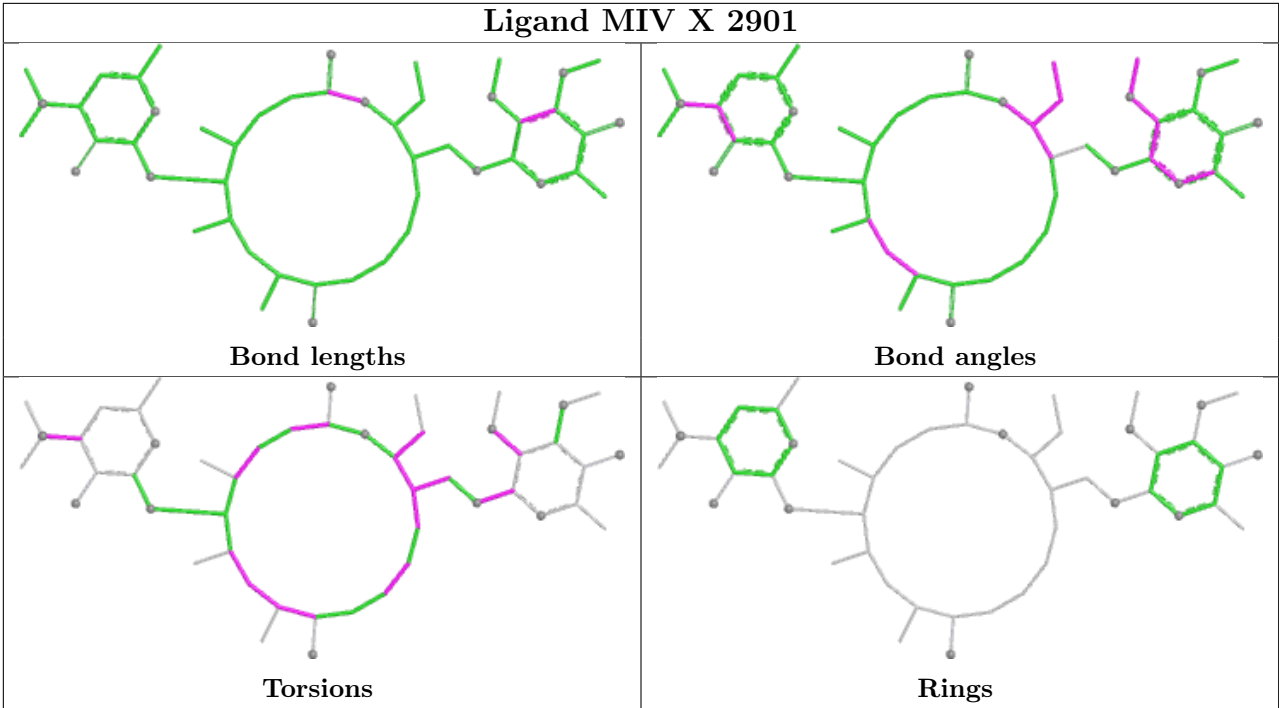
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Mol	Chain	Res	Type	Atoms
31	X	3166	SPD	N1-C2-C3-C4
31	X	3166	SPD	N6-C7-C8-C9
29	X	2901	MIV	C22-C23-C24-O5
29	X	2901	MIV	C2-C1-C28-C25
31	X	3167	SPD	C7-C8-C9-N10
31	X	3170	SPD	C8-C7-N6-C5
29	X	2901	MIV	O1-C5-C6-C8
31	X	3171	SPD	C8-C7-N6-C5
31	X	3171	SPD	C2-C3-C4-C5
31	X	3168	SPD	N1-C2-C3-C4
31	V	101	SPD	C4-C5-N6-C7
29	X	2901	MIV	C6-C8-C9-C10
29	X	2901	MIV	C28-C25-C26-C27
31	X	3170	SPD	C7-C8-C9-N10
31	X	3167	SPD	C2-C3-C4-C5
31	V	101	SPD	C8-C7-N6-C5
31	V	101	SPD	N6-C7-C8-C9
29	X	2901	MIV	C6-C8-C9-C11

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 ⓘ

There are no such residues in this entry.

4.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	X	12

All 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
1	X	1522:C	O3'	1526:U	P	17.66
1	X	725:C	O3'	732:G	P	16.37
1	X	1546:C	O3'	1558:C	P	15.65
1	X	1891:C	O3'	1908:C	P	14.39
1	X	1732:U	O3'	1735:G	P	9.97
1	X	891:A	O3'	911:A	P	7.98

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	X	724:C	O3'	725:C	P	4.77

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

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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%)

All (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
3	A	101	GLU	9.7
4	B	135	HIS	9.6
3	A	21	PHE	9.0
26	1	24	THR	8.9
28	3	40	GLU	8.8
10	I	24	GLY	8.7
13	L	56	SER	8.6
2	Y	42	U	8.6
3	A	99	ASP	8.6
10	I	103	ASN	8.4
10	I	72	TYR	8.2
19	R	43	ASP	8.0
3	A	12	SER	7.8
7	E	123	PHE	7.8
4	B	206	ALA	7.7
3	A	97	TYR	7.7
10	I	49	PHE	7.6
10	I	50	GLU	7.6
6	D	72	LYS	7.6
15	N	91	ASN	7.5
10	I	57	ILE	7.3
20	S	93	GLU	7.3
5	C	92	ASP	7.2
7	E	120	GLY	7.2
1	X	2270	U	7.2
10	I	115	SER	7.2
3	A	42	GLY	7.1

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Mol	Chain	Res	Type	RSRZ
4	B	139	GLY	7.0
1	X	251	C	6.9
1	X	1072	U	6.9
6	D	133	LYS	6.9
22	U	35	THR	6.9
6	D	94	GLU	6.8
3	A	98	ALA	6.8
3	A	272	THR	6.8
3	A	224	SER	6.7
5	C	91	TYR	6.7
3	A	37	LEU	6.6
2	Y	43	G	6.6
16	O	6	GLN	6.6
20	S	68	ALA	6.6
6	D	153	ASP	6.6
19	R	68	GLY	6.5
6	D	92	ARG	6.5
22	U	25	ARG	6.5
22	U	7	LEU	6.5
3	A	242	ALA	6.5
24	W	26	ARG	6.5
15	N	63	GLN	6.4
3	A	100	GLY	6.3
26	1	52	GLU	6.3
1	X	248	A	6.3
22	U	47	HIS	6.3
10	I	15	ASP	6.2
1	X	1116	U	6.2
3	A	260	ARG	6.2
26	1	35	LEU	6.2
18	Q	32	LYS	6.2
20	S	69	VAL	6.1
1	X	1507	A	6.1
15	N	89	ASP	6.1
28	3	45	GLY	6.1
3	A	19	ALA	6.1
6	D	23	SER	6.0
1	X	1095	A	6.0
9	H	20	MET	5.9
1	X	1602	G	5.9
8	G	171	LEU	5.9
13	L	30	SER	5.9

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Mol	Chain	Res	Type	RSRZ
3	A	52	ARG	5.8
22	U	46	LEU	5.8
5	C	94	THR	5.8
1	X	1516	A	5.8
7	E	5	GLY	5.8
23	V	48	ARG	5.8
11	J	82	THR	5.8
10	I	47	ALA	5.7
1	X	540	G	5.7
13	L	33	ARG	5.7
10	I	93	LEU	5.7
3	A	102	LYS	5.7
6	D	84	PRO	5.7
4	B	205	SER	5.6
1	X	1085	G	5.6
1	X	75	C	5.6
13	L	93	SER	5.6
1	X	2290	A	5.6
26	1	49	VAL	5.6
1	X	184	A	5.6
3	A	72	LYS	5.5
26	1	23	THR	5.5
1	X	1888	C	5.5
27	2	19	ARG	5.5
28	3	2	PRO	5.5
3	A	45	ASN	5.5
22	U	15	VAL	5.5
10	I	46	GLY	5.5
4	B	168	GLN	5.4
22	U	16	ASN	5.4
16	O	78	VAL	5.4
10	I	41	SER	5.3
4	B	117	MET	5.3
22	U	49	LYS	5.3
3	A	24	LEU	5.3
1	X	1117	G	5.3
1	X	1515	U	5.3
11	J	14	PHE	5.2
1	X	878	C	5.2
21	T	20	TYR	5.2
13	L	37	HIS	5.2
10	I	62	LYS	5.2

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Mol	Chain	Res	Type	RSRZ
3	A	35	GLU	5.2
6	D	122	PHE	5.2
20	S	70	GLN	5.2
1	X	1094	C	5.1
11	J	107	VAL	5.1
1	X	1792	C	5.1
3	A	50	THR	5.1
6	D	74	ILE	5.1
13	L	8	ARG	5.1
7	E	136	ILE	5.0
10	I	38	LYS	5.0
6	D	32	GLU	5.0
20	S	15	ASP	5.0
28	3	32	GLN	5.0
6	D	25	VAL	4.9
9	H	8	LEU	4.9
13	L	31	VAL	4.9
1	X	430	C	4.9
28	3	25	PHE	4.9
10	I	68	VAL	4.9
3	A	55	GLY	4.8
6	D	40	LEU	4.8
22	U	36	GLY	4.8
5	C	29	GLU	4.8
13	L	96	TYR	4.8
1	X	74	G	4.8
20	S	3	LEU	4.8
19	R	91	ALA	4.8
13	L	51	LEU	4.7
3	A	223	GLY	4.7
3	A	171	ASP	4.7
11	J	122	ALA	4.7
13	L	34	SER	4.7
1	X	250	C	4.7
9	H	1	MET	4.7
27	2	40	HIS	4.6
5	C	120	VAL	4.6
5	C	66	ASN	4.6
18	Q	57	ASN	4.6
1	X	653	G	4.6
1	X	774[A]	A	4.6
13	L	59	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
3	A	9	TYR	4.6
7	E	6	LYS	4.6
11	J	34	GLY	4.6
1	X	362	C	4.6
1	X	652	C	4.6
11	J	26	ASP	4.6
10	I	73	GLU	4.6
15	N	50	ARG	4.6
19	R	40	LEU	4.6
5	C	60	GLY	4.6
4	B	149	ARG	4.6
13	L	11	LEU	4.6
3	A	160	GLY	4.6
9	H	46	HIS	4.6
13	L	40	ALA	4.6
28	3	42	ARG	4.5
1	X	160	C	4.5
19	R	44	GLN	4.5
8	G	91	THR	4.5
28	3	39	ASP	4.5
7	E	7	GLN	4.5
3	A	240	THR	4.5
28	3	11	LYS	4.5
3	A	174	ILE	4.5
13	L	39	TYR	4.5
13	L	10	LYS	4.5
8	G	113	GLU	4.5
1	X	1920	A	4.5
22	U	20	ARG	4.5
18	Q	17	TYR	4.4
3	A	90	ALA	4.4
10	I	37	GLN	4.4
1	X	2444	C	4.4
16	O	40	VAL	4.4
6	D	152	MET	4.4
1	X	571	U	4.4
17	P	121	THR	4.4
1	X	1073	G	4.4
22	U	45	ASN	4.4
3	A	229	VAL	4.4
21	T	18	PRO	4.4
13	L	32	TYR	4.4

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Mol	Chain	Res	Type	RSRZ
26	1	40	TYR	4.4
15	N	90	LEU	4.3
1	X	1063	C	4.3
6	D	155	THR	4.3
3	A	57	GLY	4.3
10	I	56	LEU	4.3
1	X	1887	G	4.3
18	Q	31	PRO	4.3
3	A	71	ASP	4.3
1	X	2467	A	4.3
26	1	21	TYR	4.3
1	X	2359	U	4.3
13	L	38	ILE	4.3
26	1	17	GLY	4.3
10	I	35	LYS	4.3
3	A	239	ARG	4.3
19	R	39	ALA	4.3
3	A	59	LYS	4.2
11	J	123	GLY	4.2
3	A	76	ASN	4.2
9	H	12	ASP	4.2
17	P	118	LYS	4.2
20	S	92	VAL	4.2
6	D	119	PRO	4.2
23	V	51	ALA	4.2
22	U	63	SER	4.2
16	O	83	ARG	4.2
10	I	65	PHE	4.2
3	A	254	THR	4.2
28	3	8	LYS	4.2
1	X	429	C	4.2
22	U	29	GLY	4.2
1	X	427	C	4.2
1	X	981	C	4.2
7	E	140	LEU	4.1
19	R	56	LYS	4.1
1	X	225	G	4.1
1	X	263	G	4.1
7	E	121	VAL	4.1
22	U	14	VAL	4.1
20	S	83	PHE	4.1
22	U	61	TRP	4.1

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Mol	Chain	Res	Type	RSRZ
20	S	81	VAL	4.1
22	U	60	VAL	4.1
3	A	150	GLY	4.1
6	D	62	LEU	4.1
1	X	2361	G	4.1
4	B	155	ARG	4.1
3	A	228	PRO	4.1
10	I	33	GLY	4.0
21	T	24	LYS	4.0
13	L	35	SER	4.0
11	J	119	PHE	4.0
28	3	16	ILE	4.0
11	J	37	ALA	4.0
2	Y	44	C	4.0
3	A	238	GLY	4.0
22	U	58	LYS	4.0
13	L	20	THR	4.0
26	1	18	THR	4.0
1	X	431	G	4.0
28	3	63	PRO	4.0
1	X	408	U	4.0
8	G	129	HIS	4.0
1	X	272	U	3.9
6	D	93	GLY	3.9
22	U	73	GLY	3.9
6	D	71	LYS	3.9
1	X	278	G	3.9
6	D	20	PHE	3.9
13	L	54	ALA	3.9
20	S	65	LEU	3.9
3	A	259	THR	3.9
4	B	140	SER	3.9
13	L	9	ARG	3.9
3	A	221	GLN	3.9
1	X	1384	G	3.9
1	X	76	C	3.9
6	D	69	LYS	3.9
24	W	22	ALA	3.9
7	E	52	VAL	3.9
22	U	40	ARG	3.9
3	A	54	ILE	3.9
20	S	19	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
5	C	133	PHE	3.9
15	N	25	TRP	3.9
3	A	46	ARG	3.9
13	L	99	ARG	3.9
5	C	193	LEU	3.9
21	T	13	GLY	3.8
17	P	124	ILE	3.8
1	X	424	G	3.8
1	X	1850	G	3.8
26	1	20	PHE	3.8
1	X	70	A	3.8
22	U	44	ALA	3.8
1	X	2004	U	3.8
3	A	151	LYS	3.8
3	A	64	ILE	3.8
3	A	236	GLY	3.8
16	O	23	GLU	3.8
18	Q	27	PHE	3.8
19	R	14	LEU	3.8
8	G	78	ASP	3.8
15	N	84	LYS	3.8
1	X	420	C	3.8
3	A	43	ARG	3.8
3	A	147	LEU	3.8
4	B	136	ARG	3.8
20	S	14	LEU	3.8
10	I	95	ALA	3.8
4	B	144	ARG	3.8
6	D	13	ARG	3.8
5	C	23	ASN	3.7
13	L	95	LYS	3.7
7	E	135	GLY	3.7
1	X	1084	A	3.7
1	X	245	C	3.7
11	J	17	ARG	3.7
10	I	20	GLY	3.7
3	A	149	PRO	3.7
11	J	75	VAL	3.7
3	A	167	GLY	3.7
10	I	45	LYS	3.7
15	N	88	ILE	3.7
4	B	138	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
22	U	17	SER	3.7
26	1	22	TYR	3.7
20	S	169	VAL	3.7
1	X	926	C	3.7
9	H	7	ARG	3.7
1	X	699	G	3.6
1	X	2328	G	3.6
28	3	49	VAL	3.6
1	X	1753	A	3.6
26	1	43	VAL	3.6
26	1	37	LEU	3.6
28	3	44	LYS	3.6
1	X	2280	A	3.6
11	J	41	ALA	3.6
6	D	67	ILE	3.6
22	U	19	ILE	3.6
15	N	7	GLY	3.6
26	1	27	ASN	3.6
5	C	134	ILE	3.6
1	X	2271	C	3.6
8	G	104	THR	3.6
3	A	58	HIS	3.6
5	C	161	ALA	3.6
6	D	136	LEU	3.6
10	I	60	LEU	3.6
7	E	122	THR	3.6
1	X	1099	A	3.5
1	X	1912	G	3.5
1	X	2466	G	3.5
1	X	1517	C	3.5
3	A	137	PRO	3.5
8	G	43	VAL	3.5
11	J	100	PRO	3.5
27	2	14	LYS	3.5
3	A	226	MET	3.5
1	X	667	U	3.5
21	T	55	ARG	3.5
24	W	7	ARG	3.5
26	1	25	THR	3.5
15	N	57	PHE	3.5
26	1	47	HIS	3.5
3	A	68	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
3	A	237	GLU	3.5
20	S	29	ASN	3.5
28	3	64	ARG	3.5
8	G	164	GLN	3.5
11	J	23	LYS	3.5
13	L	97	HIS	3.5
1	X	185	C	3.5
1	X	246	C	3.5
1	X	1508	G	3.5
7	E	60	LYS	3.5
19	R	28	LYS	3.5
26	1	32	GLN	3.5
14	M	102	ALA	3.5
1	X	273	U	3.5
1	X	1015	U	3.5
19	R	69	GLN	3.5
21	T	73	GLY	3.5
28	3	60	LEU	3.5
27	2	10	ARG	3.5
6	D	157	VAL	3.4
19	R	88	THR	3.4
3	A	225	ALA	3.4
13	L	52	ALA	3.4
5	C	96	PRO	3.4
11	J	36	ILE	3.4
6	D	46	ASP	3.4
7	E	153	LYS	3.4
1	X	1409	U	3.4
21	T	22	GLY	3.4
13	L	58	ALA	3.4
6	D	30	ARG	3.4
15	N	97	ASP	3.4
14	M	88	VAL	3.4
13	L	60	LYS	3.4
3	A	250	TRP	3.4
3	A	84	TYR	3.4
9	H	55	VAL	3.4
13	L	100	VAL	3.4
15	N	40	LEU	3.4
15	N	95	LEU	3.4
19	R	67	GLY	3.4
4	B	160	MET	3.4

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Mol	Chain	Res	Type	RSRZ
1	X	1921	A	3.4
5	C	61	GLN	3.4
1	X	2570	C	3.4
8	G	139	ARG	3.4
10	I	63	ARG	3.4
1	X	742	G	3.4
1	X	1098	G	3.4
26	1	34	LYS	3.4
7	E	68	THR	3.4
18	Q	55	THR	3.4
10	I	66	ASN	3.3
3	A	51	SER	3.3
3	A	91	ARG	3.3
10	I	59	ARG	3.3
16	O	76	SER	3.3
6	D	143	TYR	3.3
22	U	26	ALA	3.3
8	G	75	ILE	3.3
19	R	113	THR	3.3
22	U	42	GLN	3.3
16	O	1	MET	3.3
6	D	144	ASP	3.3
1	X	1319	C	3.3
1	X	2199	C	3.3
3	A	96	HIS	3.3
8	G	168	THR	3.3
17	P	29	LYS	3.3
20	S	153	LYS	3.3
1	X	2370	G	3.3
3	A	74	GLY	3.3
16	O	98	ILE	3.3
18	Q	47	GLY	3.3
22	U	37	ILE	3.3
3	A	38	PRO	3.3
3	A	121	PRO	3.3
3	A	253	PRO	3.3
10	I	34	HIS	3.3
27	2	12	ARG	3.3
19	R	57	ASN	3.3
3	A	251	GLY	3.3
7	E	83	TYR	3.3
10	I	61	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
1	X	270	G	3.3
1	X	1066	G	3.3
1	X	2078	G	3.3
28	3	7	HIS	3.3
20	S	86	VAL	3.3
27	2	23	LYS	3.3
2	Y	15	A	3.3
28	3	4	MET	3.3
1	X	1885	C	3.3
2	Y	29	C	3.3
3	A	83	GLU	3.3
10	I	43	ALA	3.3
13	L	53	ALA	3.3
15	N	62	ILE	3.3
22	U	64	ALA	3.3
13	L	19	THR	3.2
25	Z	11	THR	3.2
27	2	1	MET	3.2
3	A	77	ALA	3.2
1	X	1062	G	3.2
10	I	44	GLY	3.2
1	X	2381	A	3.2
5	C	56	ARG	3.2
15	N	12	ARG	3.2
9	H	54	SER	3.2
10	I	14	LYS	3.2
27	2	46	ASP	3.2
6	D	90	THR	3.2
3	A	30	GLU	3.2
11	J	112	GLU	3.2
6	D	161	LYS	3.2
20	S	88	TYR	3.2
28	3	46	LYS	3.2
1	X	190	A	3.2
1	X	2279	G	3.2
20	S	94	VAL	3.2
1	X	520	C	3.2
1	X	2788	C	3.2
20	S	167	THR	3.2
3	A	49	ILE	3.2
23	V	17	GLU	3.2
8	G	40	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
7	E	33	LEU	3.2
7	E	8	PRO	3.2
6	D	3	GLN	3.2
6	D	132	ILE	3.2
1	X	1050	G	3.2
1	X	1104	G	3.2
1	X	2007	G	3.2
3	A	56	GLY	3.2
1	X	85	C	3.2
7	E	64	LEU	3.2
17	P	32	ARG	3.2
28	3	31	HIS	3.2
12	K	1	MET	3.2
7	E	34	THR	3.2
1	X	390	U	3.1
25	Z	8	LYS	3.1
28	3	47	GLY	3.1
1	X	2758	A	3.1
1	X	2453	C	3.1
21	T	36	ILE	3.1
10	I	58	ALA	3.1
22	U	8	THR	3.1
22	U	34	THR	3.1
6	D	123	ASP	3.1
13	L	44	ASP	3.1
18	Q	93	GLY	3.1
1	X	1357	U	3.1
2	Y	123	U	3.1
13	L	89	PHE	3.1
22	U	74	PRO	3.1
28	3	30	ARG	3.1
1	X	247	A	3.1
6	D	148	LYS	3.1
18	Q	12	ILE	3.1
2	Y	2	C	3.1
8	G	71	THR	3.1
18	Q	2	SER	3.1
1	X	30	G	3.1
1	X	271	G	3.1
1	X	2269	G	3.1
3	A	20	ASP	3.1
1	X	2192	U	3.1

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Mol	Chain	Res	Type	RSRZ
3	A	204	ILE	3.1
10	I	121	HIS	3.1
3	A	256	GLY	3.1
20	S	157	GLY	3.1
1	X	2205	C	3.1
10	I	18	ARG	3.1
23	V	44	ARG	3.1
1	X	965	G	3.1
1	X	382	U	3.1
10	I	75	VAL	3.1
10	I	118	VAL	3.1
6	D	134	GLU	3.1
23	V	30	PHE	3.1
1	X	116	A	3.1
6	D	22	TYR	3.1
1	X	1364	C	3.0
1	X	2089	C	3.0
1	X	2360	C	3.0
3	A	271	VAL	3.0
5	C	166	TRP	3.0
26	1	12	MET	3.0
20	S	51	LEU	3.0
1	X	249	A	3.0
1	X	1106	A	3.0
1	X	2189	A	3.0
3	A	186	HIS	3.0
11	J	109	GLY	3.0
16	O	11	GLN	3.0
23	V	36	GLN	3.0
1	X	1086	C	3.0
1	X	1795	C	3.0
28	3	43	GLY	3.0
8	G	30	LYS	3.0
13	L	87	VAL	3.0
5	C	123	PHE	3.0
14	M	11	GLU	3.0
7	E	134	SER	3.0
15	N	74	MET	3.0
18	Q	51	ILE	3.0
1	X	1071	U	3.0
1	X	2380	U	3.0
1	X	1266	G	3.0

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Mol	Chain	Res	Type	RSRZ
1	X	2174	G	3.0
3	A	6	TYR	3.0
6	D	120	ASN	3.0
7	E	113	VAL	3.0
17	P	68	VAL	3.0
1	X	96	C	3.0
13	L	55	SER	3.0
27	2	45	SER	3.0
3	A	172	TYR	3.0
1	X	86	U	3.0
1	X	183	U	3.0
8	G	97	ASP	3.0
20	S	114	ASP	3.0
19	R	84	VAL	3.0
19	R	104	VAL	3.0
28	3	33	ASN	3.0
1	X	1057	A	3.0
1	X	1367	A	3.0
1	X	2520	A	3.0
3	A	61	LEU	3.0
5	C	89	ARG	3.0
1	X	226	C	3.0
8	G	44	VAL	3.0
13	L	92	GLY	3.0
17	P	97	VAL	3.0
1	X	2385	U	3.0
1	X	2706	U	3.0
22	U	65	ASN	3.0
15	N	60	LEU	2.9
4	B	137	ARG	2.9
1	X	252	G	2.9
4	B	128	SER	2.9
1	X	71	A	2.9
1	X	435	A	2.9
1	X	665	A	2.9
6	D	85	VAL	2.9
11	J	137	VAL	2.9
13	L	48	GLY	2.9
18	Q	23	GLY	2.9
1	X	391	C	2.9
19	R	54	ILE	2.9
28	3	58	MET	2.9

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Mol	Chain	Res	Type	RSRZ
16	O	7	THR	2.9
8	G	137	LYS	2.9
19	R	78	ALA	2.9
22	U	41	VAL	2.9
10	I	42	GLY	2.9
1	X	2015	G	2.9
1	X	1349	A	2.9
1	X	1582	A	2.9
19	R	13	LYS	2.9
20	S	100	THR	2.9
21	T	74	LYS	2.9
1	X	434	C	2.9
1	X	927	C	2.9
1	X	2170	C	2.9
7	E	112	PRO	2.9
20	S	20	ALA	2.9
26	1	33	ALA	2.9
13	L	94	TYR	2.9
3	A	60	ARG	2.9
20	S	134	LEU	2.9
1	X	1356	G	2.9
5	C	173	ALA	2.9
6	D	118	ASN	2.9
13	L	104	ALA	2.9
10	I	106	VAL	2.9
1	X	1466	C	2.9
1	X	1687	C	2.9
1	X	1023	U	2.9
1	X	1922	U	2.9
3	A	180	GLY	2.9
3	A	82	ILE	2.9
9	H	56	LYS	2.9
23	V	52	GLN	2.9
15	N	87	ASN	2.9
5	C	169	VAL	2.9
13	L	91	ARG	2.9
1	X	732	G	2.9
1	X	1179	A	2.9
13	L	42	ILE	2.9
1	X	1513	U	2.8
1	X	2197	U	2.8
8	G	101	THR	2.8

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Mol	Chain	Res	Type	RSRZ
22	U	12	ASN	2.8
3	A	47	GLY	2.8
3	A	67	PHE	2.8
7	E	174	GLY	2.8
6	D	66	ILE	2.8
17	P	117	ILE	2.8
22	U	51	ILE	2.8
1	X	123	A	2.8
1	X	425	A	2.8
1	X	2194	A	2.8
2	Y	28	A	2.8
3	A	73	SER	2.8
7	E	119	ALA	2.8
10	I	117	ALA	2.8
1	X	1913	G	2.8
2	Y	120	G	2.8
6	D	38	GLU	2.8
11	J	11	ARG	2.8
19	R	46	VAL	2.8
11	J	88	LYS	2.8
21	T	42	GLY	2.8
12	K	87	TYR	2.8
22	U	24	ALA	2.8
22	U	50	ALA	2.8
26	1	14	SER	2.8
15	N	33	ARG	2.8
5	C	99	VAL	2.8
1	X	1180	A	2.8
1	X	1603	A	2.8
7	E	89	LEU	2.8
1	X	872	G	2.8
1	X	1765	C	2.8
1	X	2386	G	2.8
1	X	2610	G	2.8
5	C	2	ALA	2.8
20	S	121	GLN	2.8
3	A	13	ARG	2.8
15	N	55	ARG	2.8
7	E	133	VAL	2.8
13	L	36	LYS	2.8
19	R	86	PRO	2.8
17	P	106	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
22	U	59	THR	2.8
23	V	24	GLU	2.8
6	D	50	ILE	2.8
3	A	234	GLY	2.8
6	D	116	GLY	2.8
1	X	167	A	2.8
1	X	394	U	2.8
1	X	1154	A	2.8
1	X	2476	A	2.8
7	E	37	TYR	2.8
16	O	74	TYR	2.8
1	X	1087	C	2.8
1	X	1411	C	2.8
1	X	1700	C	2.8
1	X	2329	C	2.8
28	3	51	ALA	2.8
11	J	44	LYS	2.8
1	X	192	G	2.8
1	X	383	G	2.8
7	E	43	VAL	2.8
18	Q	13	SER	2.8
13	L	50	THR	2.8
22	U	43	ARG	2.7
17	P	69	ALA	2.7
1	X	118	U	2.7
1	X	159	A	2.7
1	X	775	U	2.7
1	X	2409	A	2.7
1	X	2714	A	2.7
8	G	107	GLN	2.7
10	I	19	VAL	2.7
11	J	110	VAL	2.7
25	Z	28	PRO	2.7
23	V	37	LEU	2.7
1	X	1115	C	2.7
1	X	1692	C	2.7
1	X	2343	C	2.7
8	G	124	GLU	2.7
6	D	41	GLY	2.7
1	X	516	G	2.7
1	X	1322	G	2.7
1	X	1352	G	2.7

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Mol	Chain	Res	Type	RSRZ
1	X	2006	G	2.7
25	Z	53	ASP	2.7
6	D	129	ASN	2.7
15	N	52	ASN	2.7
25	Z	13	LYS	2.7
28	3	36	LYS	2.7
12	K	3	HIS	2.7
7	E	36	PRO	2.7
11	J	74	PRO	2.7
9	H	18	GLU	2.7
1	X	1320	A	2.7
3	A	23	GLY	2.7
22	U	28	GLY	2.7
6	D	80	ARG	2.7
16	O	13	ARG	2.7
3	A	255	LYS	2.7
18	Q	35	LYS	2.7
1	X	1877	C	2.7
12	K	97	ILE	2.7
12	K	80	MET	2.7
3	A	217	ARG	2.7
12	K	56	LYS	2.7
21	T	72	LYS	2.7
1	X	642	A	2.7
1	X	964	A	2.7
5	C	43	ALA	2.7
1	X	2443	C	2.7
5	C	84	PHE	2.7
6	D	114	PHE	2.7
11	J	57	ARG	2.7
15	N	44	THR	2.7
28	3	17	THR	2.7
1	X	1284	G	2.7
1	X	1832	G	2.7
16	O	12	ALA	2.7
19	R	82	ALA	2.7
1	X	1467	U	2.7
16	O	25	LEU	2.7
20	S	166	LEU	2.7
3	A	44	ASN	2.7
1	X	2636	A	2.6
6	D	2	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
6	D	141	ILE	2.6
7	E	69	ARG	2.6
14	M	44	ARG	2.6
3	A	168	LYS	2.6
7	E	101	LYS	2.6
1	X	863	C	2.6
1	X	1581	C	2.6
8	G	146	THR	2.6
11	J	111	THR	2.6
13	L	65	THR	2.6
7	E	173	ALA	2.6
1	X	2071	G	2.6
9	H	19	ILE	2.6
8	G	72	PRO	2.6
25	Z	15	LYS	2.6
27	2	35	ARG	2.6
1	X	1564	U	2.6
1	X	2592	U	2.6
1	X	1509	A	2.6
2	Y	27	A	2.6
19	R	106	VAL	2.6
21	T	21	LEU	2.6
1	X	2519	C	2.6
6	D	97	TYR	2.6
3	A	262	LYS	2.6
6	D	95	ARG	2.6
14	M	117	ILE	2.6
11	J	105	PHE	2.6
4	B	121	ASN	2.6
5	C	8	GLY	2.6
12	K	49	GLU	2.6
1	X	1067	G	2.6
1	X	1148	G	2.6
1	X	1589	G	2.6
7	E	16	THR	2.6
11	J	35	LEU	2.6
13	L	79	ALA	2.6
18	Q	16	ALA	2.6
1	X	2169	A	2.6
1	X	2265	A	2.6
15	N	59	ARG	2.6
3	A	212	SER	2.6

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Mol	Chain	Res	Type	RSRZ
6	D	73	SER	2.6
27	2	26	SER	2.6
20	S	78	PRO	2.6
1	X	1049	C	2.6
7	E	59	GLN	2.6
5	C	194	GLU	2.6
4	B	72	VAL	2.6
5	C	54	THR	2.6
15	N	6	THR	2.6
23	V	55	THR	2.6
26	1	44	ALA	2.6
5	C	68	ARG	2.6
13	L	64	LYS	2.6
15	N	58	ARG	2.6
20	S	73	LYS	2.6
1	X	84	G	2.6
1	X	1074	G	2.6
1	X	2166	G	2.6
1	X	2362	G	2.6
1	X	2481	G	2.6
1	X	2503	G	2.6
1	X	1796	A	2.6
26	1	41	ASP	2.6
7	E	50	LEU	2.6
17	P	57	LEU	2.6
12	K	89	GLU	2.6
3	A	3	VAL	2.6
5	C	39	ARG	2.6
12	K	12	ARG	2.6
20	S	168	VAL	2.6
21	T	41	ARG	2.6
23	V	43	VAL	2.6
28	3	34	THR	2.6
4	B	95	ILE	2.5
8	G	100	TYR	2.5
9	H	21	CYS	2.5
14	M	12	LEU	2.5
1	X	1228	G	2.5
1	X	1390	G	2.5
1	X	1889	G	2.5
3	A	258	LYS	2.5
15	N	34	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
22	U	11	LYS	2.5
22	U	27	ASP	2.5
6	D	165	GLU	2.5
8	G	59	ALA	2.5
1	X	4	C	2.5
1	X	102	C	2.5
4	B	84	PHE	2.5
3	A	233	HIS	2.5
1	X	1037	U	2.5
1	X	1481	U	2.5
1	X	2080	U	2.5
15	N	23	GLY	2.5
17	P	119	LYS	2.5
6	D	26	MET	2.5
1	X	158	A	2.5
1	X	2468	G	2.5
5	C	117	LEU	2.5
8	G	90	LEU	2.5
3	A	235	GLY	2.5
10	I	25	GLY	2.5
20	S	175	ARG	2.5
6	D	24	SER	2.5
11	J	22	ALA	2.5
17	P	129	ALA	2.5
21	T	61	ALA	2.5
1	X	259	U	2.5
1	X	1101	U	2.5
7	E	38	ASN	2.5
19	R	11	ASN	2.5
3	A	257	LEU	2.5
15	N	83	LEU	2.5
19	R	102	LYS	2.5
1	X	199	A	2.5
1	X	1096	A	2.5
1	X	1952	A	2.5
3	A	241	GLY	2.5
6	D	39	GLY	2.5
15	N	73	GLY	2.5
7	E	139	GLN	2.5
1	X	122	G	2.5
1	X	157	G	2.5
1	X	776	G	2.5

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Mol	Chain	Res	Type	RSRZ
11	J	118	ALA	2.5
28	3	37	SER	2.5
1	X	1111	C	2.5
1	X	2072	C	2.5
2	Y	45	C	2.5
1	X	1804	U	2.5
4	B	118	LYS	2.5
4	B	145	LYS	2.5
6	D	55	LYS	2.5
20	S	63	PRO	2.5
27	2	7	PRO	2.5
8	G	108	GLY	2.5
24	W	17	VAL	2.5
13	L	86	GLN	2.5
10	I	39	SER	2.4
12	K	14	SER	2.4
20	S	54	ILE	2.4
1	X	253	A	2.4
1	X	1088	A	2.4
1	X	1260	A	2.4
1	X	1693	A	2.4
20	S	18	MET	2.4
11	J	61	ARG	2.4
28	3	12	ARG	2.4
1	X	1045	G	2.4
1	X	1082	G	2.4
1	X	1815	G	2.4
1	X	2183	C	2.4
1	X	2230	G	2.4
1	X	2353	G	2.4
3	A	132	PRO	2.4
22	U	30	VAL	2.4
5	C	168	SER	2.4
11	J	92	GLU	2.4
12	K	114	GLU	2.4
20	S	170	SER	2.4
15	N	41	ASN	2.4
1	X	1081	A	2.4
1	X	1954	A	2.4
2	Y	101	A	2.4
7	E	46	ASP	2.4
17	P	125	THR	2.4

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Mol	Chain	Res	Type	RSRZ
4	B	53	PRO	2.4
11	J	16	GLY	2.4
1	X	422	C	2.4
1	X	219	G	2.4
1	X	1368	G	2.4
1	X	1369	G	2.4
1	X	1563	U	2.4
1	X	1565	G	2.4
1	X	2051	U	2.4
7	E	53	GLU	2.4
14	M	46	ARG	2.4
6	D	16	LEU	2.4
5	C	20	PRO	2.4
7	E	42	THR	2.4
20	S	155	PRO	2.4
5	C	26	VAL	2.4
10	I	133	VAL	2.4
27	2	44	VAL	2.4
5	C	49	ALA	2.4
8	G	85	ALA	2.4
11	J	80	ALA	2.4
1	X	2705	A	2.4
2	Y	60	A	2.4
15	N	8	ILE	2.4
8	G	65	LYS	2.4
11	J	12	LYS	2.4
19	R	66	GLN	2.4
15	N	101	ARG	2.4
18	Q	62	ARG	2.4
1	X	1112	U	2.4
1	X	1531	C	2.4
1	X	2274	C	2.4
1	X	2291	U	2.4
19	R	83	LEU	2.4
21	T	62	LEU	2.4
21	T	63	SER	2.4
1	X	50	G	2.4
1	X	395	G	2.4
1	X	1435	G	2.4
1	X	1963	G	2.4
4	B	22	PRO	2.4
19	R	99	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
3	A	41	GLY	2.4
5	C	12	GLY	2.4
20	S	144	GLY	2.4
4	B	151	TYR	2.4
6	D	106	ILE	2.4
7	E	10	ALA	2.4
11	J	93	TYR	2.4
27	2	30	ILE	2.4
3	A	264	LYS	2.4
7	E	27	LYS	2.4
3	A	70	ARG	2.4
10	I	81	GLN	2.4
1	X	512	A	2.4
1	X	833	A	2.4
1	X	956	A	2.4
1	X	1314	A	2.4
1	X	2037	A	2.4
7	E	110	SER	2.4
4	B	126	PRO	2.4
16	O	22	VAL	2.4
28	3	55	TRP	2.4
1	X	1327	C	2.3
6	D	162	THR	2.3
19	R	89	GLY	2.3
6	D	117	ILE	2.3
18	Q	53	ILE	2.3
28	3	3	LYS	2.3
1	X	2408	G	2.3
1	X	2433	G	2.3
1	X	2746	G	2.3
6	D	79	LEU	2.3
6	D	103	LEU	2.3
23	V	39	GLN	2.3
22	U	57	VAL	2.3
3	A	232	PRO	2.3
1	X	693	A	2.3
1	X	1288	A	2.3
1	X	1406	A	2.3
5	C	64	THR	2.3
7	E	22	GLY	2.3
7	E	152	ARG	2.3
8	G	63	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
10	I	13	ARG	2.3
11	J	15	ARG	2.3
24	W	24	GLY	2.3
1	X	398	C	2.3
11	J	72	ASP	2.3
21	T	15	ASP	2.3
3	A	33	LEU	2.3
3	A	53	PHE	2.3
13	L	29	LEU	2.3
1	X	2216	G	2.3
1	X	2532	G	2.3
7	E	151	VAL	2.3
24	W	45	LYS	2.3
28	3	26	LYS	2.3
10	I	105	PRO	2.3
6	D	31	ILE	2.3
19	R	23	ILE	2.3
28	3	41	ILE	2.3
13	L	107	ALA	2.3
18	Q	83	ALA	2.3
5	C	93	TYR	2.3
23	V	53	LEU	2.3
27	2	8	ASN	2.3
1	X	747	A	2.3
1	X	1278	A	2.3
1	X	2289	A	2.3
2	Y	63	A	2.3
1	X	1392	U	2.3
1	X	114	C	2.3
1	X	1283	C	2.3
1	X	1506	C	2.3
1	X	2206	C	2.3
3	A	208	LYS	2.3
7	E	17	VAL	2.3
11	J	133	VAL	2.3
15	N	53	LYS	2.3
24	W	40	VAL	2.3
28	3	21	LYS	2.3
11	J	20	GLY	2.3
24	W	29	GLY	2.3
3	A	140	ALA	2.3
28	3	50	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	X	1033	G	2.3
1	X	1735	G	2.3
15	N	45	TYR	2.3
27	2	5	TYR	2.3
23	V	14	PHE	2.3
6	D	63	GLN	2.3
21	T	49	GLN	2.3
3	A	27	LYS	2.3
1	X	436	A	2.3
4	B	163	GLU	2.3
8	G	125	ARG	2.3
3	A	128	GLY	2.3
3	A	156	ALA	2.3
5	C	67	ALA	2.3
5	C	191	ALA	2.3
28	3	38	GLY	2.3
1	X	258	C	2.3
1	X	1616	C	2.3
2	Y	81	C	2.3
4	B	134	TRP	2.3
6	D	149	THR	2.3
3	A	138	VAL	2.3
8	G	150	VAL	2.3
10	I	99	VAL	2.3
6	D	140	GLU	2.2
1	X	227	G	2.2
1	X	487	G	2.2
1	X	594	G	2.2
1	X	2425	G	2.2
2	Y	117	G	2.2
22	U	78	ILE	2.2
8	G	133	GLY	2.2
9	H	45	ALA	2.2
1	X	260	U	2.2
1	X	1453	A	2.2
1	X	2224	U	2.2
1	X	2428	U	2.2
1	X	2452	U	2.2
1	X	2784	A	2.2
11	J	121	LEU	2.2
8	G	156	HIS	2.2
6	D	128	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
7	E	150	LYS	2.2
1	X	280	C	2.2
1	X	750	C	2.2
1	X	975	C	2.2
1	X	1623	C	2.2
1	X	1836	C	2.2
1	X	2374	C	2.2
2	Y	5	C	2.2
13	L	71	VAL	2.2
4	B	94	ASP	2.2
17	P	98	ASP	2.2
3	A	36	ALA	2.2
24	W	43	MET	2.2
1	X	614	G	2.2
1	X	713	G	2.2
1	X	741	G	2.2
1	X	877	G	2.2
1	X	1323	G	2.2
1	X	1666	G	2.2
1	X	1849	G	2.2
17	P	123	HIS	2.2
1	X	840	U	2.2
3	A	63	ARG	2.2
1	X	618	A	2.2
5	C	44	SER	2.2
9	H	97	VAL	2.2
21	T	38	VAL	2.2
27	2	41	GLN	2.2
6	D	127	ASN	2.2
4	B	98	GLU	2.2
6	D	154	ILE	2.2
13	L	109	GLU	2.2
1	X	1103	C	2.2
1	X	1575	C	2.2
1	X	1830	C	2.2
1	X	2195	C	2.2
5	C	121	ASP	2.2
11	J	101	GLY	2.2
14	M	104	LEU	2.2
15	N	2	PRO	2.2
15	N	42	ALA	2.2
20	S	5	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
23	V	28	LEU	2.2
17	P	19	LYS	2.2
18	Q	28	TRP	2.2
10	I	26	THR	2.2
10	I	70	THR	2.2
14	M	45	THR	2.2
20	S	87	THR	2.2
9	H	44	TYR	2.2
20	S	66	VAL	2.2
16	O	15	SER	2.2
1	X	2223	U	2.2
1	X	2298	U	2.2
1	X	636	G	2.2
1	X	1223	G	2.2
1	X	1226	A	2.2
1	X	1432	G	2.2
1	X	2317	G	2.2
3	A	181	GLU	2.2
3	A	29	PRO	2.2
20	S	131	PRO	2.2
27	2	13	ALA	2.2
7	E	94	PHE	2.2
11	J	7	ARG	2.2
1	X	1169	C	2.2
1	X	2849	C	2.2
5	C	30	VAL	2.2
6	D	35	VAL	2.2
15	N	94	VAL	2.2
5	C	4	ILE	2.2
14	M	2	GLN	2.2
6	D	130	LEU	2.2
10	I	98	LEU	2.2
3	A	87	ASN	2.2
18	Q	15	LYS	2.2
1	X	2222	U	2.2
1	X	2483	U	2.2
2	Y	54	U	2.2
25	Z	38	GLY	2.2
26	1	42	PRO	2.2
3	A	28	ARG	2.2
8	G	53	ARG	2.2
14	M	101	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
9	H	57	ASP	2.2
1	X	1068	A	2.2
1	X	1574	A	2.2
1	X	2190	A	2.2
1	X	950	G	2.2
1	X	1360	G	2.2
1	X	1880	G	2.2
1	X	2424	G	2.2
1	X	2750	G	2.2
5	C	45	THR	2.1
5	C	157	THR	2.1
3	A	206	LEU	2.1
5	C	53	LYS	2.1
8	G	134	MET	2.1
8	G	170	PRO	2.1
1	X	1434	U	2.1
1	X	2456	U	2.1
16	O	84	THR	2.1
1	X	101	A	2.1
1	X	304	A	2.1
1	X	1203	A	2.1
1	X	1585	A	2.1
1	X	2566	A	2.1
7	E	115	ILE	2.1
22	U	67	LEU	2.1
1	X	2341	G	2.1
1	X	573	C	2.1
1	X	2056	C	2.1
1	X	2082	C	2.1
3	A	8	PRO	2.1
3	A	125	PRO	2.1
3	A	152	GLY	2.1
5	C	65	GLY	2.1
6	D	82	GLY	2.1
7	E	118	PRO	2.1
8	G	138	GLY	2.1
6	D	138	PHE	2.1
19	R	81	VAL	2.1
1	X	1454	U	2.1
1	X	1601	U	2.1
3	A	95	LEU	2.1
4	B	5	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
4	B	133	LYS	2.1
14	M	103	LYS	2.1
28	3	19	THR	2.1
20	S	74	ARG	2.1
23	V	47	ARG	2.1
8	G	76	GLN	2.1
9	H	11	ALA	2.1
11	J	114	GLN	2.1
3	A	243	GLY	2.1
21	T	45	PHE	2.1
4	B	192	ASN	2.1
1	X	388	G	2.1
1	X	1533	G	2.1
1	X	2083	G	2.1
1	X	2200	G	2.1
1	X	2773	G	2.1
2	Y	53	G	2.1
1	X	1090	C	2.1
1	X	2565	C	2.1
4	B	8	LYS	2.1
20	S	80	HIS	2.1
22	U	76	LYS	2.1
5	C	142	LEU	2.1
28	3	62	LEU	2.1
13	L	18	ARG	2.1
10	I	96	TYR	2.1
11	J	19	THR	2.1
15	N	92	ARG	2.1
18	Q	22	ARG	2.1
12	K	94	TYR	2.1
21	T	58	THR	2.1
1	X	302	U	2.1
1	X	561	U	2.1
1	X	1618	U	2.1
1	X	1766	U	2.1
1	X	2323	U	2.1
2	Y	10	U	2.1
6	D	124	GLY	2.1
9	H	37	GLY	2.1
19	R	53	VAL	2.1
20	S	116	VAL	2.1
1	X	879	A	2.1

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Mol	Chain	Res	Type	RSRZ
1	X	1583	A	2.1
1	X	2182	A	2.1
2	Y	59	A	2.1
17	P	37	LYS	2.1
21	T	12	ASN	2.1
3	A	105	ILE	2.1
7	E	51	LEU	2.1
15	N	65	ILE	2.1
26	1	8	ILE	2.1
5	C	76	THR	2.1
6	D	17	MET	2.1
8	G	45	ASP	2.1
17	P	30	TYR	2.1
1	X	426	C	2.1
1	X	1791	C	2.1
1	X	1808	C	2.1
1	X	2499	C	2.1
1	X	59	G	2.1
1	X	119	G	2.1
1	X	983	G	2.1
1	X	1847	G	2.1
11	J	115	ALA	2.1
13	L	22	ALA	2.1
5	C	70	GLY	2.1
11	J	63	GLY	2.1
1	X	974	U	2.0
1	X	1748	U	2.0
3	A	5	LYS	2.0
8	G	159	SER	2.0
5	C	170	LEU	2.0
8	G	110	LEU	2.0
8	G	116	ARG	2.0
1	X	402	A	2.0
1	X	795	A	2.0
1	X	1510	A	2.0
1	X	1671	A	2.0
2	Y	41	A	2.0
3	A	25	THR	2.0
8	G	69	ASP	2.0
15	N	76	TYR	2.0
20	S	33	ALA	2.0
9	H	38	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
13	L	98	GLY	2.0
27	2	18	PHE	2.0
1	X	113	C	2.0
1	X	537	C	2.0
1	X	1060	C	2.0
1	X	1083	C	2.0
1	X	1522	C	2.0
1	X	2454	C	2.0
15	N	19	LYS	2.0
11	J	28	VAL	2.0
1	X	111	G	2.0
1	X	389	G	2.0
1	X	2330	G	2.0
1	X	2447	G	2.0
1	X	2474	G	2.0
2	Y	46	G	2.0
3	A	133	LEU	2.0
17	P	73	ASN	2.0
20	S	141	MET	2.0
16	O	3	ALA	2.0
28	3	6	THR	2.0
7	E	164	PHE	2.0
10	I	112	GLY	2.0
17	P	59	PHE	2.0
22	U	22	GLY	2.0
26	1	19	GLY	2.0
4	B	32	PRO	2.0
7	E	55	PRO	2.0
16	O	79	GLN	2.0
18	Q	10	PRO	2.0
1	X	195	A	2.0
1	X	922	A	2.0
1	X	2737	A	2.0
1	X	2779	A	2.0
1	X	2866	A	2.0
22	U	53	GLU	2.0
6	D	91	LEU	2.0
7	E	67	LEU	2.0
1	X	1615	C	2.0
1	X	1797	C	2.0
1	X	1844	C	2.0

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

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

5.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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
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

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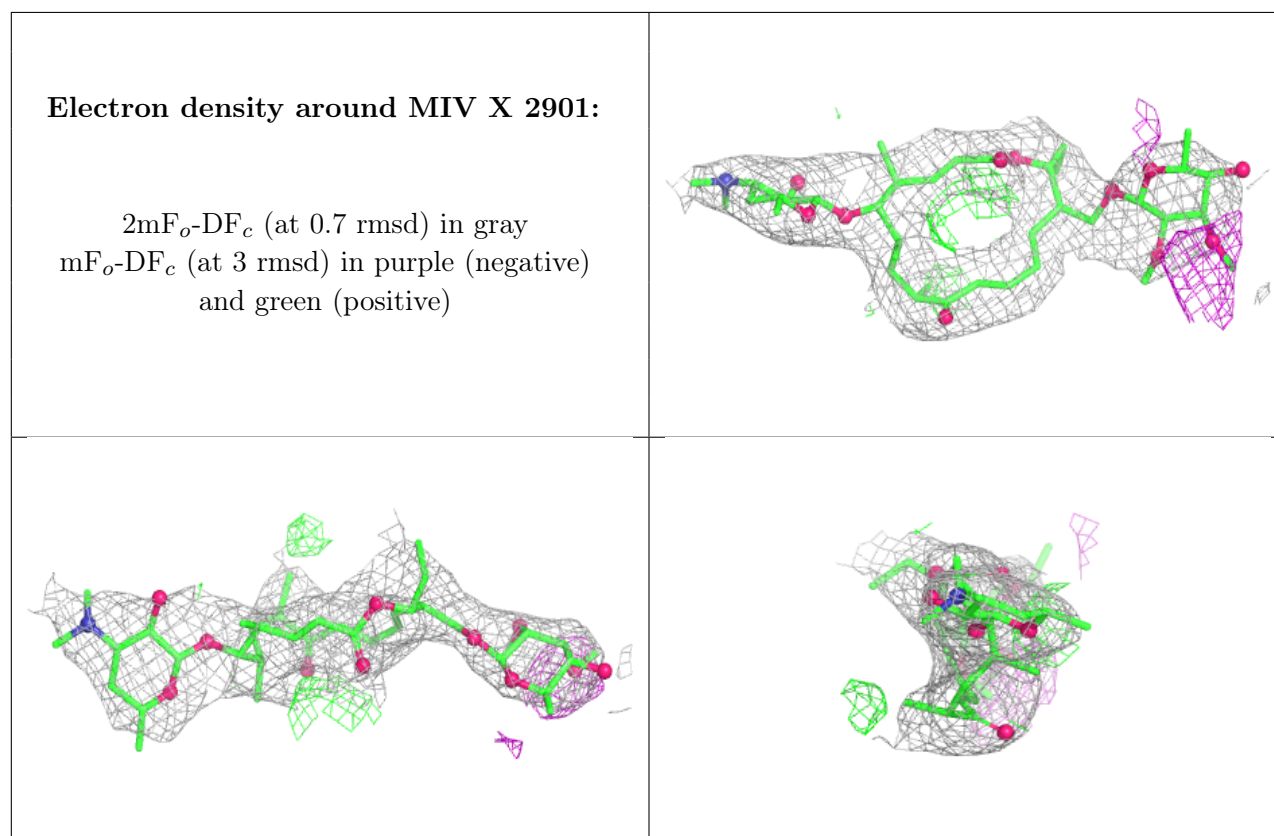
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MG	X	3100	1/1	0.91	0.09	77,77,77,77	0
30	MG	X	2946	1/1	0.92	0.33	51,51,51,51	0
30	MG	X	3132	1/1	0.92	0.20	88,88,88,88	0
30	MG	X	3007	1/1	0.92	0.20	71,71,71,71	0
30	MG	X	3021	1/1	0.92	0.47	73,73,73,73	0
30	MG	X	3113	1/1	0.92	0.36	55,55,55,55	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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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 ⓘ

There are no such residues in this entry.