



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 04:08 PM UTC

PDB ID : 4WFB / pdb_00004wfb
Title : The crystal structure of the large ribosomal subunit of Staphylococcus aureus in complex with BC-3205
Authors : Eyal, Z.; Matzov, D.; Krupkin, M.; Wekselman, I.; Zimmerman, E.; Rozenberg, H.; Bashan, A.; Yonath, A.E.
Deposited on : 2014-09-14
Resolution : 3.43 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (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

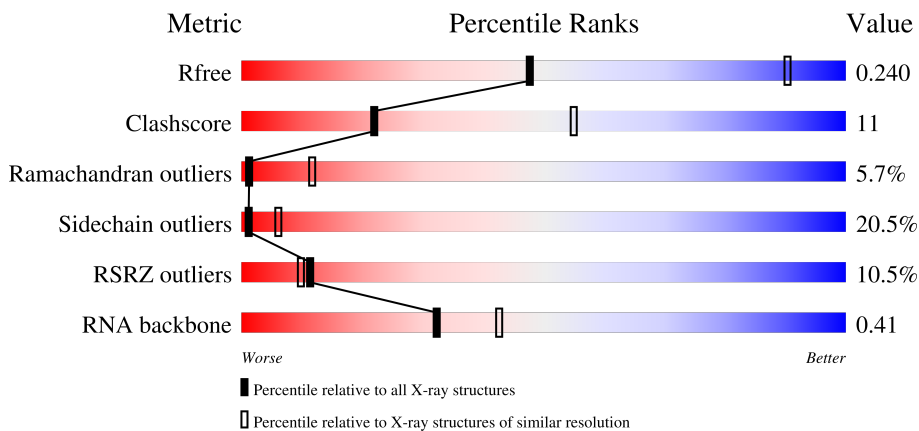
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.43 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	1736 (3.50-3.38)
Clashscore	190562	1808 (3.50-3.38)
Ramachandran outliers	187476	1776 (3.50-3.38)
Sidechain outliers	187428	1777 (3.50-3.38)
RSRZ outliers	180081	1736 (3.50-3.38)
RNA backbone	3983	1170 (3.88-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	X	2923	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 49%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 34%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: grey;"></div> </div>
2	Y	114	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 43%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 54%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 0%; height: 10px; background-color: grey;"></div> </div>
3	A	277	<div style="display: flex; align-items: center;"> <div style="width: 20%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 61%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 30%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 0%; height: 10px; background-color: grey;"></div> </div>

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Mol	Chain	Length	Quality of chain
4	B	220	14% 52% 33% 12% .
5	C	207	7% 52% 34% 10% .
6	D	179	18% 68% 9% . 22%
7	E	178	17% 61% 25% . 12%
8	G	145	17% 54% 37% 7% .
9	H	122	10% 65% 32% .
10	I	146	29% 45% 33% 11% . 10%
11	J	144	15% 44% 44% 5% . 6%
12	K	122	10% 49% 39% 10% .
13	L	119	15% 61% 28% . 8%
14	M	116	13% 52% 34% 8% . 6%
15	N	118	8% 62% 33% . .
16	O	102	% 59% 30% 10% .
17	P	117	8% 56% 32% 6% 7%
18	Q	91	24% 64% 30% . . .
19	R	105	22% 52% 30% 10% . 5%
20	S	217	3% 47% 19% 6% 28%
21	T	94	14% 55% 18% 6% 20%
22	U	62	56% 61% 10% 29%
23	V	69	17% 68% 22% . 6%
24	W	59	12% 56% 36% 5% .
25	Z	58	7% 40% 29% 7% 24%
26	2	45	51% 38% 9% .
27	3	66	12% 62% 27% . 9%
28	4	37	54% 59% 27% 14%

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	MPD	X	3003	-	-	-	X
31	MG	X	3069	-	-	-	X
31	MG	X	3089	-	-	-	X
31	MG	X	3167	-	-	-	X
34	SPD	C	302	-	-	-	X
34	SPD	X	3427	-	-	-	X
34	SPD	X	3428	-	-	-	X
34	SPD	X	3434	-	-	X	-
35	EOH	X	3436	-	-	-	X
35	EOH	X	3438	-	-	-	X
35	EOH	X	3442	-	-	-	X
35	EOH	Y	208	-	-	-	X

2 Entry composition [i](#)

There are 35 unique types of molecules in this entry. The entry contains 81184 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 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	X	2707	58034	25908	10634	18785	2707	0	0	0

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	Y	114	2430	1086	436	794	114	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	271	1608	975	318	311	4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	B	215	1547	969	290	283	5	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	C	199	1318	817	254	245	2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	D	139	707	421	139	146	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	E	156	934	571	176	186	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	G	145	1083	679	203	198	3	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	H	122	824	501	161	158	4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	I	131	820	498	165	156	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	J	136	1013	650	184	175	4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	K	119	886	543	172	170	1	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
13	L	110	678	416	135	127	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
14	M	109	822	520	163	139	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	N	116	932	587	188	153	4	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
16	O	101	738	468	135	135	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
17	P	109	823	515	157	149	2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
18	Q	89	572	353	105	111	3	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
19	R	100	607	368	117	121	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
20	S	157	1020	639	180	199	2	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
21	T	75	539	336	105	98	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
22	U	44	246	149	51	46	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
23	V	65	459	283	85	91	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
24	W	57	413	255	79	79	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
25	Z	44	342	209	72	58	3	0	0	0

- Molecule 26 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
26	2	44	348	211	83	53	1	0	0	0

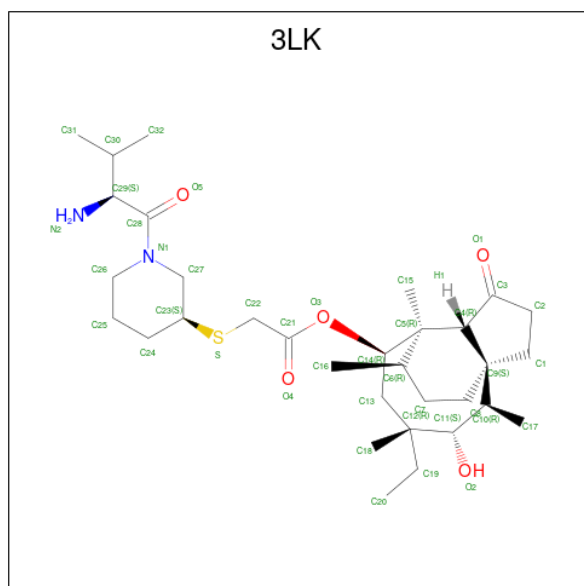
- Molecule 27 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
27	3	60	405	249	82	72	2	0	0	0

- Molecule 28 is a protein called 50S ribosomal protein L36.

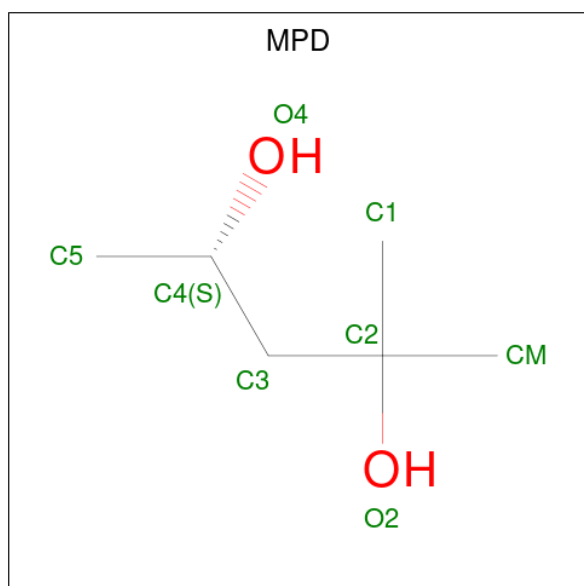
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
28	4	37	245	149	51	41	4	0	0	0

- Molecule 29 is BC-3205 (CCD ID: 3LK) (formula: $C_{32}H_{54}N_2O_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
29	X	1	40	32	2	5	1	0	0

- Molecule 30 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	X	1	Total C O 8 6 2	0	0
30	X	1	Total C O 8 6 2	0	0
30	X	1	Total C O 8 6 2	0	0
30	X	1	Total C O 8 6 2	0	0
30	X	1	Total C O 8 6 2	0	0
30	X	1	Total C O 8 6 2	0	0
30	X	1	Total C O 8 6 2	0	0
30	X	1	Total C O 8 6 2	0	0
30	X	1	Total C O 8 6 2	0	0
30	X	1	Total C O 8 6 2	0	0
30	X	1	Total C O 8 6 2	0	0
30	X	1	Total C O 8 6 2	0	0
30	X	1	Total C O 8 6 2	0	0
30	X	1	Total C O 8 6 2	0	0
30	X	1	Total C O 8 6 2	0	0
30	X	1	Total C O 8 6 2	0	0
30	X	1	Total C O 8 6 2	0	0
30	X	1	Total C O 8 6 2	0	0

- Molecule 31 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	X	100	Total Mg 100 100	0	0
31	Y	4	Total Mg 4 4	0	0
31	A	1	Total Mg 1 1	0	0
31	B	2	Total Mg 2 2	0	0
31	C	1	Total Mg 1 1	0	0

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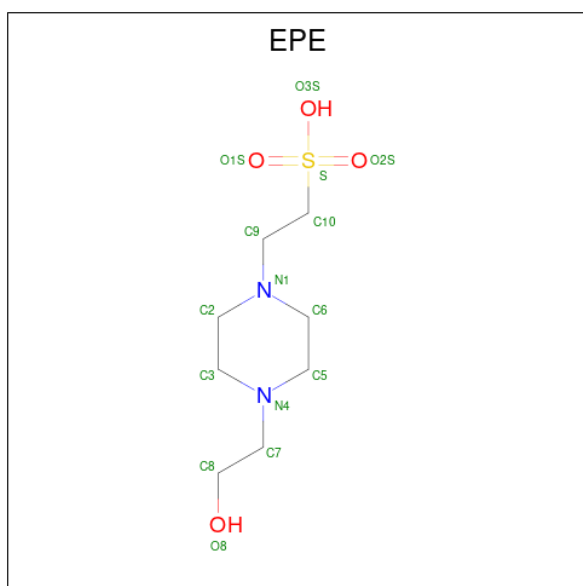
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	E	1	Total Mg 1 1	0	0
31	G	1	Total Mg 1 1	0	0
31	O	1	Total Mg 1 1	0	0

- Molecule 32 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	X	306	Total Mn 306 306	0	0
32	Y	3	Total Mn 3 3	0	0
32	A	1	Total Mn 1 1	0	0
32	R	1	Total Mn 1 1	0	0

- Molecule 33 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C₈H₁₈N₂O₄S).



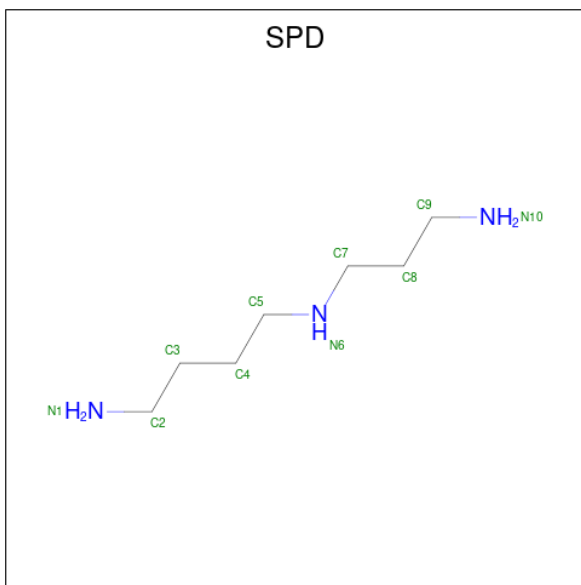
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	X	1	Total C N O S 15 8 2 4 1	0	0
33	X	1	Total C N O S 15 8 2 4 1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
33	X	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
33	X	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 34 is SPERMIDINE (CCD ID: SPD) (formula: C₇H₁₉N₃).



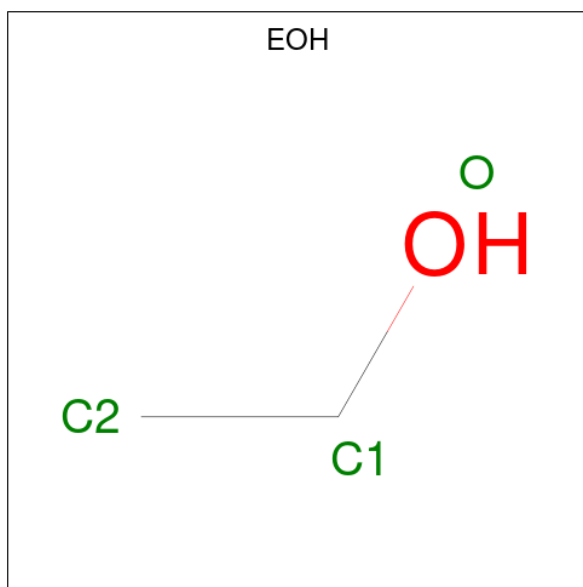
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	X	1	Total	C	N	0	0
			10	7	3		
34	X	1	Total	C	N	0	0
			10	7	3		
34	X	1	Total	C	N	0	0
			10	7	3		
34	X	1	Total	C	N	0	0
			10	7	3		
34	X	1	Total	C	N	0	0
			10	7	3		
34	X	1	Total	C	N	0	0
			10	7	3		
34	X	1	Total	C	N	0	0
			10	7	3		

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

- Molecule 35 is ETHANOL (CCD ID: EOH) (formula: C₂H₆O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	X	1	Total	C	O	0	0
			3	2	1		
35	X	1	Total	C	O	0	0
			3	2	1		
35	X	1	Total	C	O	0	0
			3	2	1		
35	X	1	Total	C	O	0	0
			3	2	1		
35	X	1	Total	C	O	0	0
			3	2	1		
35	X	1	Total	C	O	0	0
			3	2	1		
35	X	1	Total	C	O	0	0
			3	2	1		
35	X	1	Total	C	O	0	0
			3	2	1		

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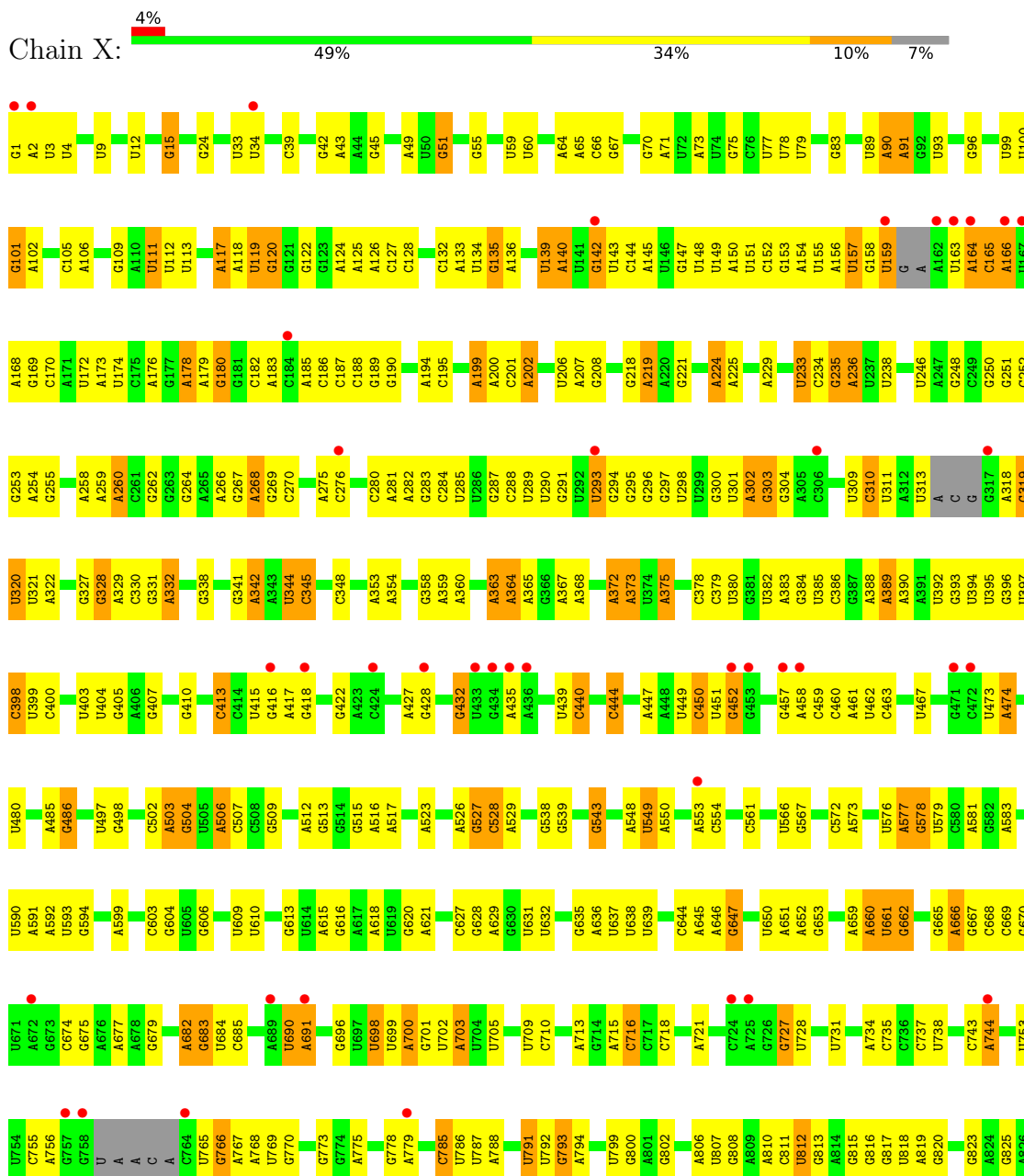
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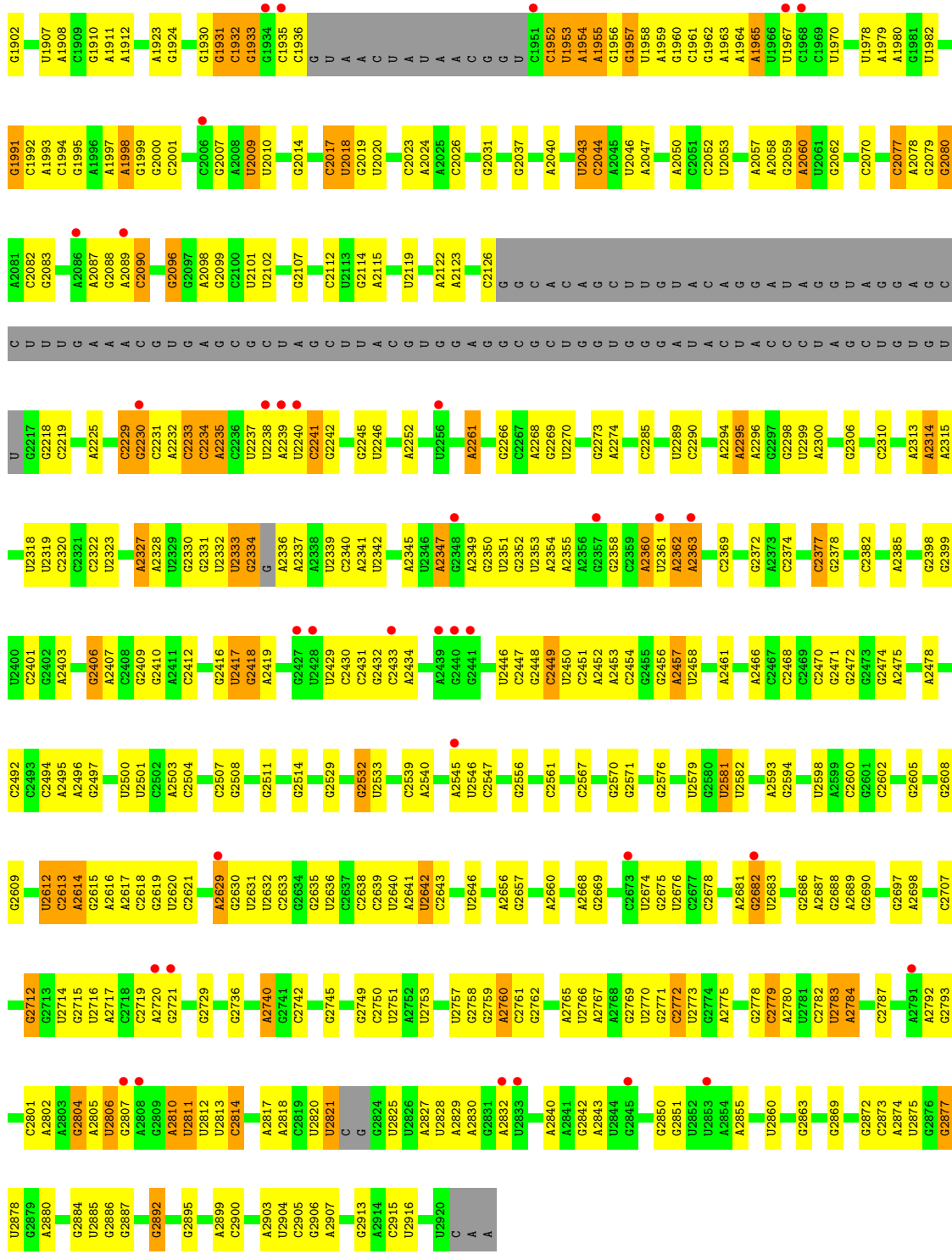
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
35	Y	1	3	2	1	0	0
35	K	1	3	2	1	0	0
35	W	1	3	2	1	0	0
35	W	1	3	2	1	0	0

3 Residue-property plots [i](#)

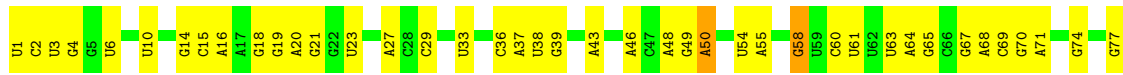
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

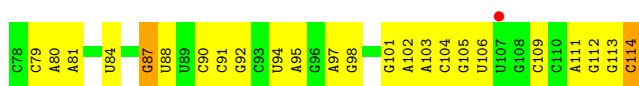
• Molecule 1: 23S rRNA



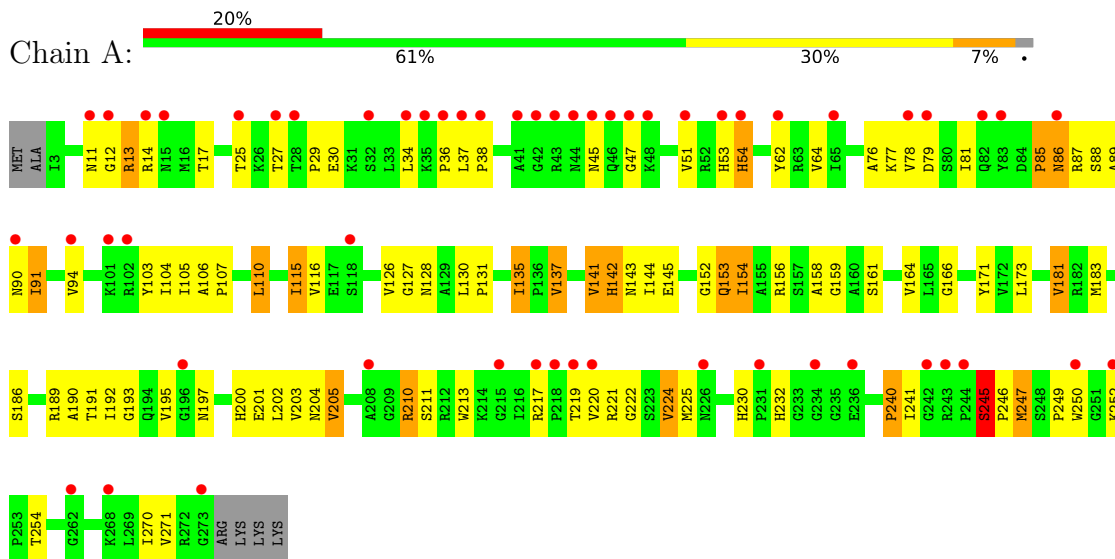


• Molecule 2: 5S rRNA

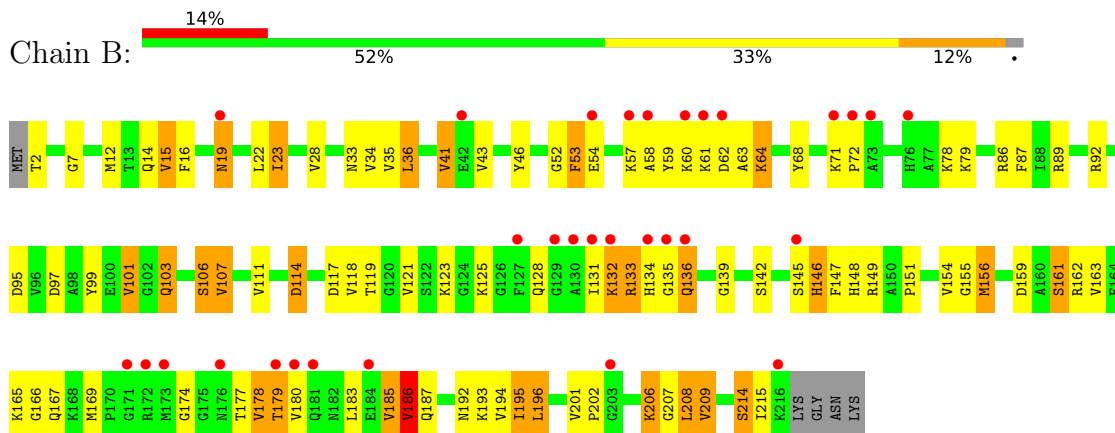




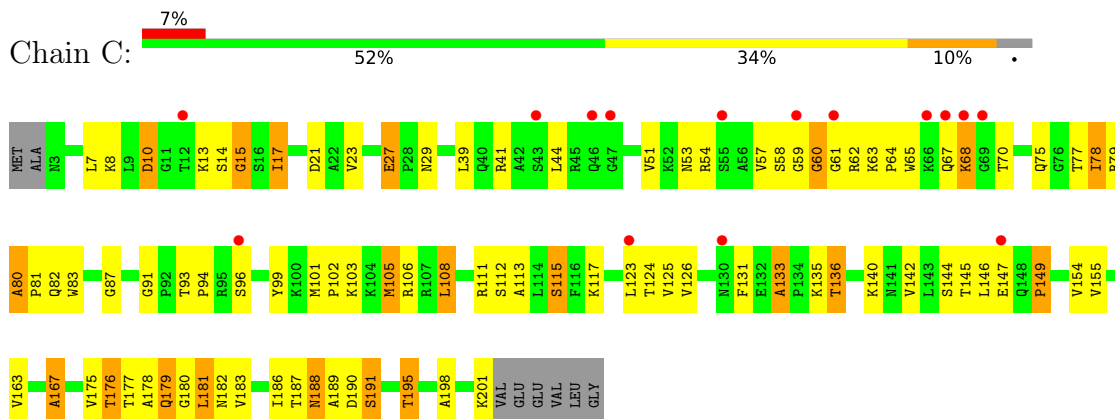
• Molecule 3: 50S ribosomal protein L2



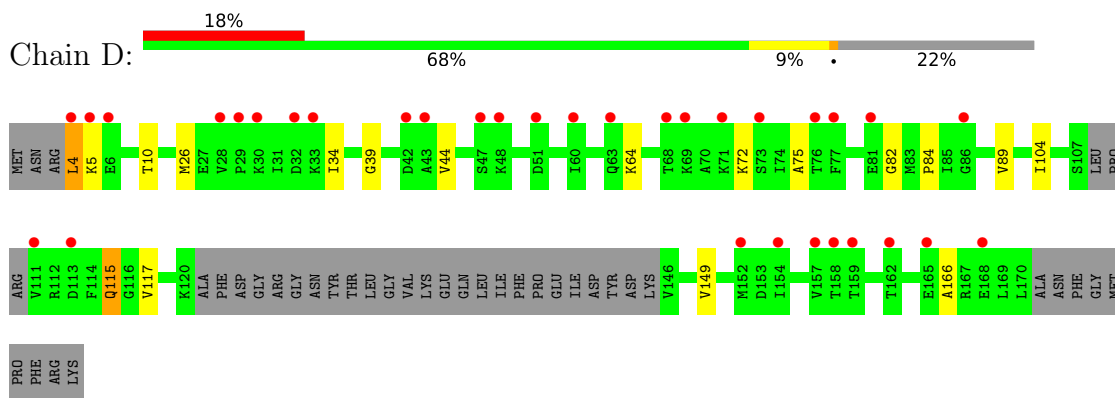
• Molecule 4: 50S ribosomal protein L3



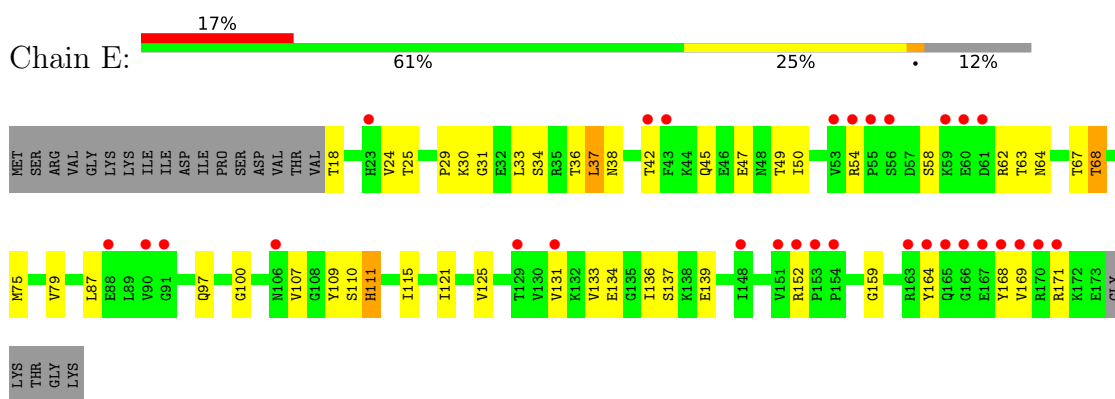
• Molecule 5: 50S ribosomal protein L4



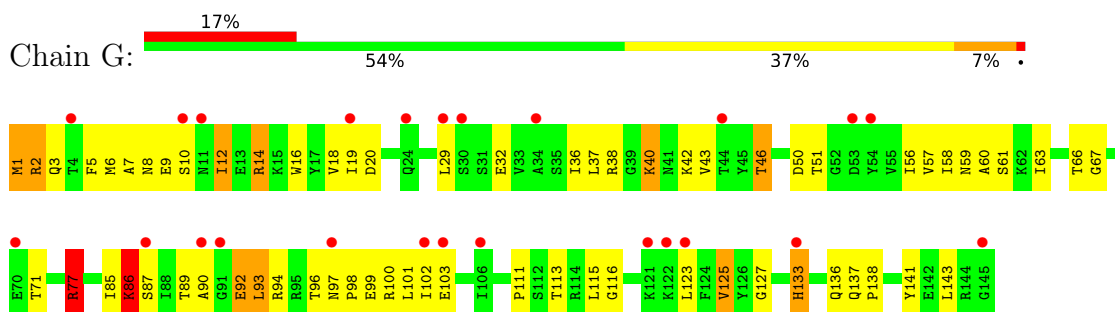
- Molecule 6: 50S ribosomal protein L5



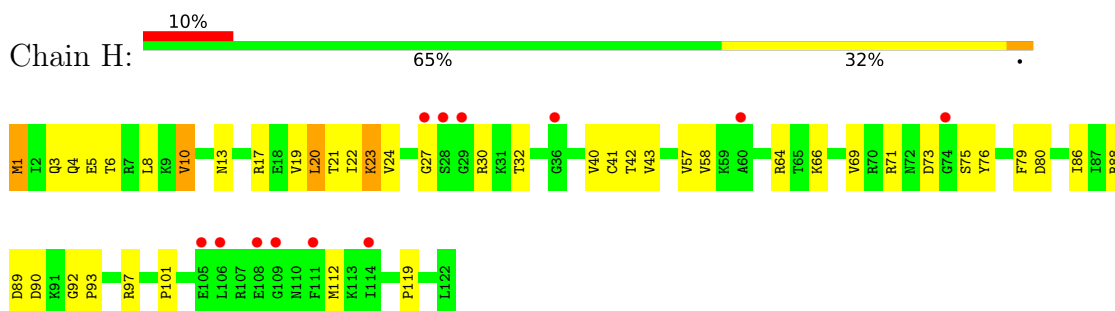
- Molecule 7: 50S ribosomal protein L6



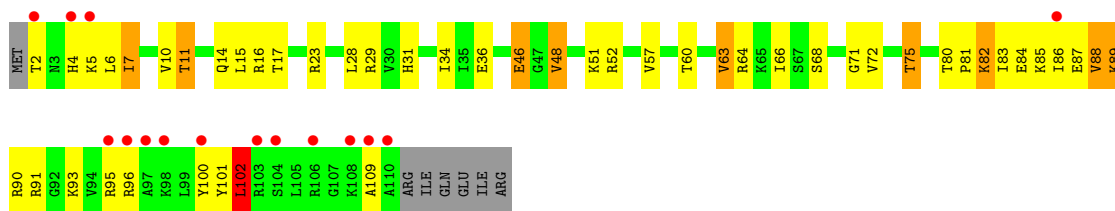
- Molecule 8: 50S ribosomal protein L13



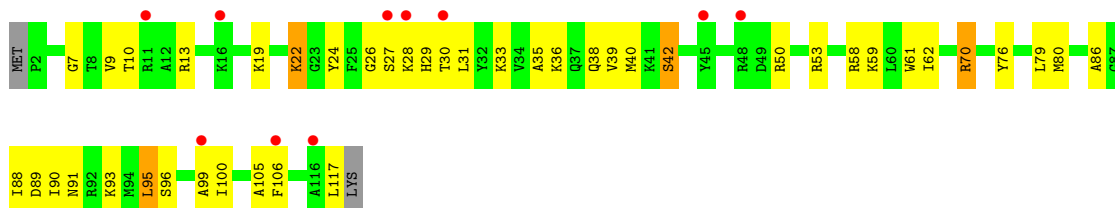
- Molecule 9: 50S ribosomal protein L14



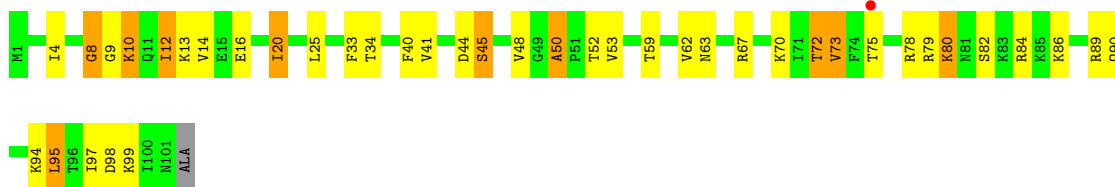
- Molecule 10: 50S ribosomal protein L15



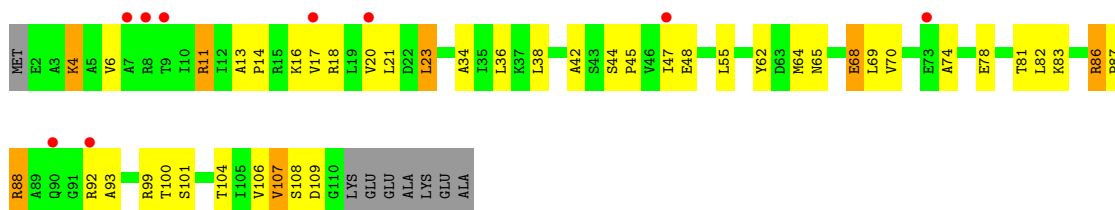
- Molecule 15: 50S ribosomal protein L20



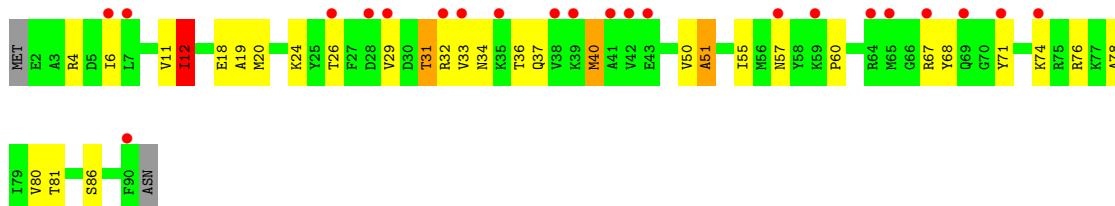
- Molecule 16: 50S ribosomal protein L21



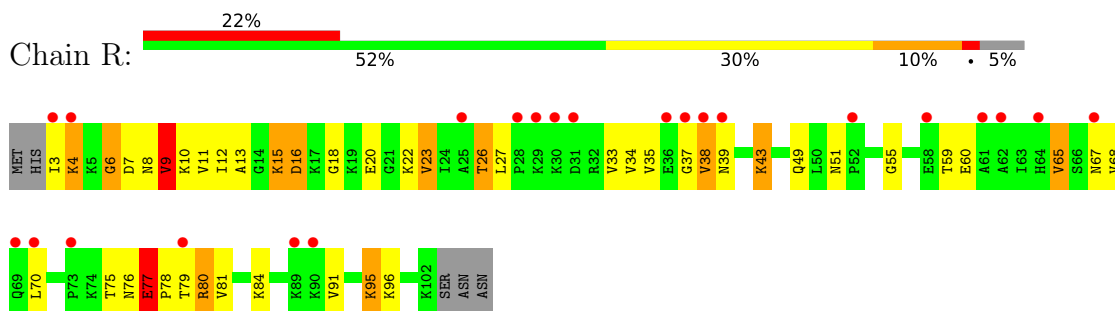
- Molecule 17: 50S ribosomal protein L22



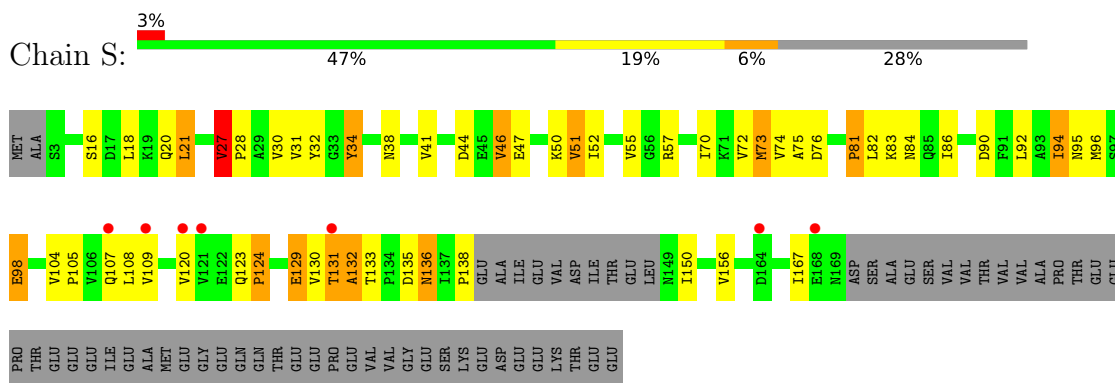
- Molecule 18: 50S ribosomal protein L23



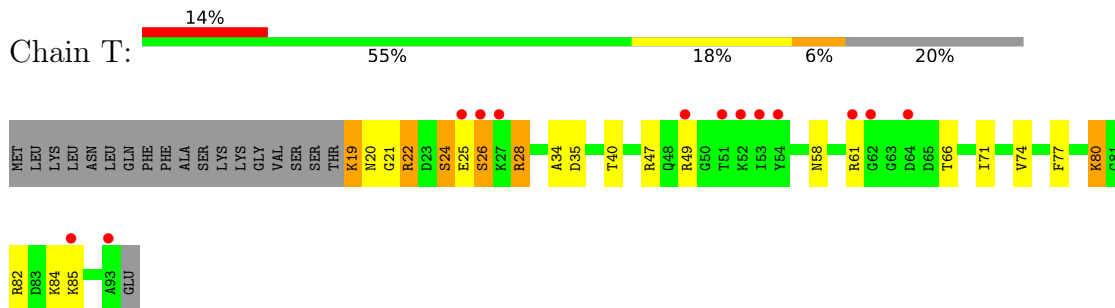
- Molecule 19: 50S ribosomal protein L24



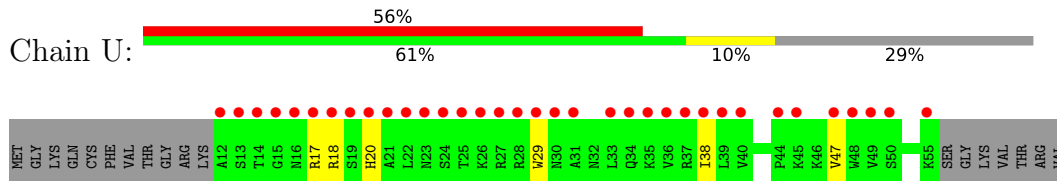
- Molecule 20: 50S ribosomal protein L25



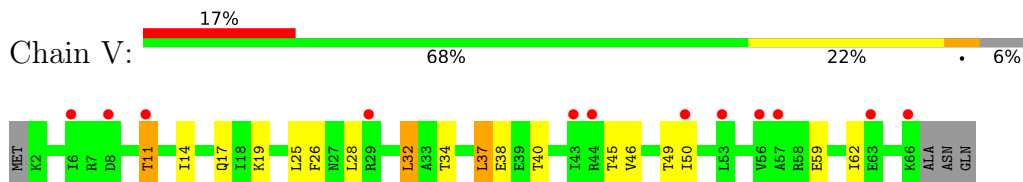
- Molecule 21: 50S ribosomal protein L27



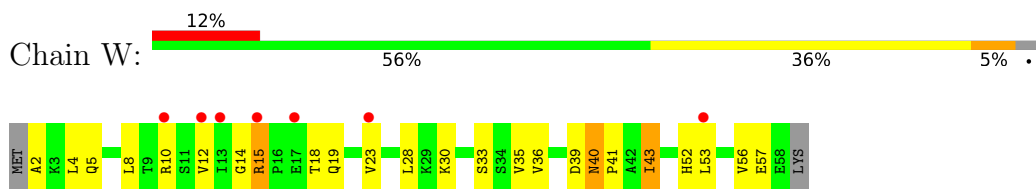
- Molecule 22: 50S ribosomal protein L28



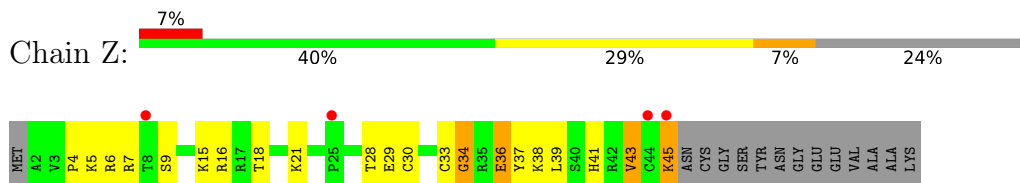
- Molecule 23: 50S ribosomal protein L29



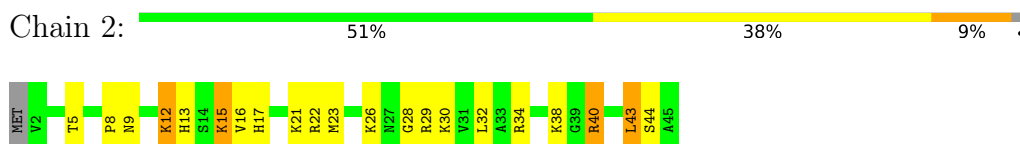
- Molecule 24: 50S ribosomal protein L30



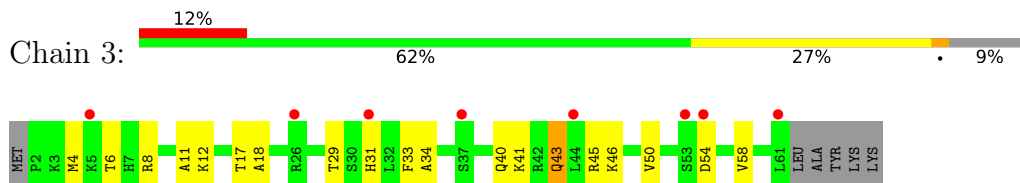
- Molecule 25: 50S ribosomal protein L32



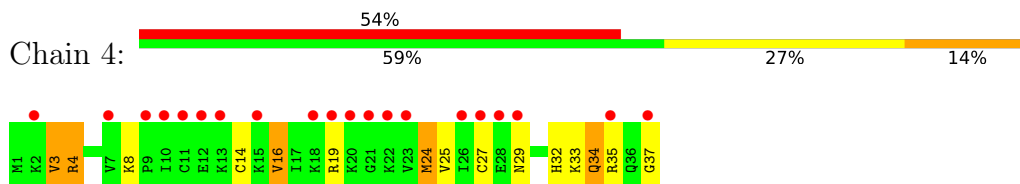
- Molecule 26: 50S ribosomal protein L34



- Molecule 27: 50S ribosomal protein L35



- Molecule 28: 50S ribosomal protein L36



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	280.92Å 280.92Å 875.59Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.54 – 3.43 49.54 – 3.43	Depositor EDS
% Data completeness (in resolution range)	91.8 (49.54-3.43) 92.3 (49.54-3.43)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 3.40Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.204 , 0.242 0.203 , 0.240	Depositor DCC
R_{free} test set	12763 reflections (4.62%)	wwPDB-VP
Wilson B-factor (Å ²)	98.3	Xtrriage
Anisotropy	0.249	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 30.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	81184	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.35% 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.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 3LK, EOH, MG, SPD, MPD, EPE, MN

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 $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	X	0.30	0/64978	0.48	0/101293
2	Y	0.27	0/2717	0.45	0/4232
3	A	0.53	0/1635	1.16	16/2256 (0.7%)
4	B	0.65	0/1570	1.16	6/2116 (0.3%)
5	C	0.65	1/1337 (0.1%)	1.12	11/1829 (0.6%)
6	D	0.45	0/704	1.05	5/973 (0.5%)
7	E	0.51	0/943	1.14	8/1301 (0.6%)
8	G	0.60	0/1105	1.10	6/1498 (0.4%)
9	H	0.54	0/830	1.02	1/1125 (0.1%)
10	I	0.73	1/827 (0.1%)	1.32	11/1120 (1.0%)
11	J	0.63	0/1037	1.17	11/1404 (0.8%)
12	K	0.60	0/889	1.09	6/1192 (0.5%)
13	L	0.50	0/683	0.98	2/935 (0.2%)
14	M	0.60	0/834	1.05	2/1125 (0.2%)
15	N	0.74	0/944	1.07	2/1252 (0.2%)
16	O	0.58	0/748	1.32	8/1007 (0.8%)
17	P	0.66	0/831	0.97	1/1122 (0.1%)
18	Q	0.51	0/577	0.99	2/791 (0.3%)
19	R	0.65	0/611	1.19	7/837 (0.8%)
20	S	0.58	0/1030	1.04	3/1412 (0.2%)
21	T	0.53	0/545	1.03	1/728 (0.1%)
22	U	0.46	0/249	0.95	0/345
23	V	0.46	0/460	0.84	0/621
24	W	0.66	0/415	1.09	4/565 (0.7%)
25	Z	0.61	0/347	1.07	3/461 (0.7%)
26	2	0.53	0/351	1.04	0/461
27	3	0.84	0/409	1.24	3/547 (0.5%)
28	4	0.58	0/246	0.92	1/330 (0.3%)
All	All	0.39	2/87852 (0.0%)	0.66	120/132878 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	B	0	2
11	J	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	I	35	HIS	CA-C	7.96	1.56	1.52
5	C	176	THR	CA-CB	5.28	1.62	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	O	50	ALA	CA-C-N	-16.64	102.62	119.76
16	O	50	ALA	C-N-CA	-16.64	102.62	119.76
7	E	152	ARG	CA-C-N	11.86	128.32	119.66
7	E	152	ARG	C-N-CA	11.86	128.32	119.66
11	J	12	GLN	N-CA-C	10.51	122.73	111.28

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	B	166	GLY	Peptide
4	B	207	GLY	Peptide
11	J	11	ARG	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	58034	0	29194	780	1
2	Y	2430	0	1229	51	0
3	A	1608	0	1202	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1547	0	1526	62	0
5	C	1318	0	1167	47	0
6	D	707	0	349	4	0
7	E	934	0	679	14	0
8	G	1083	0	1030	51	0
9	H	824	0	766	21	0
10	I	820	0	678	30	0
11	J	1013	0	993	36	0
12	K	886	0	889	32	0
13	L	678	0	547	27	0
14	M	822	0	837	30	0
15	N	932	0	997	32	0
16	O	738	0	716	20	0
17	P	823	0	866	30	0
18	Q	572	0	456	17	0
19	R	607	0	489	24	0
20	S	1020	0	868	21	0
21	T	539	0	525	15	0
22	U	246	0	147	2	0
23	V	459	0	421	11	0
24	W	413	0	414	12	0
25	Z	342	0	345	17	0
26	2	348	0	373	16	0
27	3	405	0	367	7	0
28	4	245	0	215	12	0
29	X	40	0	52	8	0
30	X	120	0	210	14	0
31	A	1	0	0	0	0
31	B	2	0	0	0	0
31	C	1	0	0	0	0
31	E	1	0	0	0	0
31	G	1	0	0	0	0
31	O	1	0	0	0	0
31	X	100	0	0	0	0
31	Y	4	0	0	0	0
32	A	1	0	0	0	0
32	R	1	0	0	0	0
32	X	306	0	0	0	0
32	Y	3	0	0	0	0
33	X	60	0	68	10	0
34	C	10	0	19	1	0
34	X	100	0	190	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	K	3	0	6	0	0
35	W	6	0	12	0	0
35	X	27	0	54	0	0
35	Y	3	0	6	0	0
All	All	81184	0	48902	1328	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

The worst 5 of 1328 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2290:C:H41	21:T:24:SER:HB3	1.23	1.02
1:X:548:A:H5''	1:X:549:U:H5'	1.51	0.92
5:C:77:THR:HG22	5:C:79:ARG:H	1.36	0.90
9:H:4:GLN:HG2	9:H:5:GLU:HG2	1.54	0.89
2:Y:80:A:H61	2:Y:91:C:H42	1.22	0.88

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:136:A:OP1	1:X:1453:G:N2[12_554]	2.17	0.03

5.3 Torsion angles [\(i\)](#)

5.3.1 Protein backbone [\(i\)](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	A	269/277 (97%)	216 (80%)	30 (11%)	23 (9%)	0 6
4	B	213/220 (97%)	181 (85%)	19 (9%)	13 (6%)	1 10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	C	197/207 (95%)	168 (85%)	18 (9%)	11 (6%)	1	12
6	D	133/179 (74%)	112 (84%)	13 (10%)	8 (6%)	1	10
7	E	154/178 (86%)	112 (73%)	30 (20%)	12 (8%)	1	7
8	G	143/145 (99%)	125 (87%)	14 (10%)	4 (3%)	4	24
9	H	120/122 (98%)	110 (92%)	7 (6%)	3 (2%)	4	25
10	I	129/146 (88%)	88 (68%)	24 (19%)	17 (13%)	0	2
11	J	134/144 (93%)	117 (87%)	10 (8%)	7 (5%)	1	13
12	K	117/122 (96%)	98 (84%)	12 (10%)	7 (6%)	1	10
13	L	108/119 (91%)	94 (87%)	10 (9%)	4 (4%)	2	19
14	M	107/116 (92%)	90 (84%)	11 (10%)	6 (6%)	1	12
15	N	114/118 (97%)	111 (97%)	2 (2%)	1 (1%)	14	45
16	O	99/102 (97%)	86 (87%)	6 (6%)	7 (7%)	1	8
17	P	107/117 (92%)	102 (95%)	5 (5%)	0	100	100
18	Q	87/91 (96%)	80 (92%)	4 (5%)	3 (3%)	3	21
19	R	98/105 (93%)	75 (76%)	14 (14%)	9 (9%)	0	5
20	S	153/217 (70%)	121 (79%)	19 (12%)	13 (8%)	0	6
21	T	73/94 (78%)	65 (89%)	5 (7%)	3 (4%)	2	17
22	U	42/62 (68%)	31 (74%)	9 (21%)	2 (5%)	2	14
23	V	63/69 (91%)	61 (97%)	1 (2%)	1 (2%)	7	33
24	W	55/59 (93%)	51 (93%)	3 (6%)	1 (2%)	6	31
25	Z	42/58 (72%)	36 (86%)	5 (12%)	1 (2%)	4	26
26	2	42/45 (93%)	39 (93%)	3 (7%)	0	100	100
27	3	58/66 (88%)	44 (76%)	7 (12%)	7 (12%)	0	3
28	4	35/37 (95%)	32 (91%)	2 (6%)	1 (3%)	3	23
All	All	2892/3215 (90%)	2445 (84%)	283 (10%)	164 (6%)	1	12

5 of 164 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	38	PRO
3	A	51	VAL
3	A	156	ARG
3	A	270	ILE
4	B	53	PHE

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	96/224 (43%)	87 (91%)	9 (9%)	8	30
4	B	150/177 (85%)	113 (75%)	37 (25%)	1	3
5	C	104/169 (62%)	78 (75%)	26 (25%)	0	3
6	D	9/158 (6%)	7 (78%)	2 (22%)	1	4
7	E	56/155 (36%)	41 (73%)	15 (27%)	0	2
8	G	104/123 (85%)	84 (81%)	20 (19%)	1	7
9	H	73/100 (73%)	60 (82%)	13 (18%)	2	9
10	I	54/112 (48%)	34 (63%)	20 (37%)	0	1
11	J	95/119 (80%)	75 (79%)	20 (21%)	1	5
12	K	85/102 (83%)	68 (80%)	17 (20%)	1	6
13	L	40/95 (42%)	31 (78%)	9 (22%)	1	4
14	M	81/102 (79%)	61 (75%)	20 (25%)	1	3
15	N	93/98 (95%)	82 (88%)	11 (12%)	5	22
16	O	69/86 (80%)	56 (81%)	13 (19%)	1	8
17	P	84/94 (89%)	72 (86%)	12 (14%)	3	16
18	Q	39/82 (48%)	32 (82%)	7 (18%)	2	9
19	R	42/90 (47%)	26 (62%)	16 (38%)	0	1
20	S	82/190 (43%)	64 (78%)	18 (22%)	1	5
21	T	48/75 (64%)	40 (83%)	8 (17%)	2	12
22	U	7/52 (14%)	6 (86%)	1 (14%)	3	16
23	V	40/62 (64%)	33 (82%)	7 (18%)	2	10
24	W	43/53 (81%)	38 (88%)	5 (12%)	5	23
25	Z	36/51 (71%)	29 (81%)	7 (19%)	1	7
26	2	34/40 (85%)	26 (76%)	8 (24%)	1	3
27	3	32/57 (56%)	27 (84%)	5 (16%)	2	13
28	4	20/35 (57%)	15 (75%)	5 (25%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1616/2701 (60%)	1285 (80%)	331 (20%)	1 6

5 of 331 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	O	95	LEU
21	T	22	ARG
17	P	81	THR
19	R	65	VAL
23	V	49	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
12	K	106	GLN
16	O	65	GLN
23	V	36	GLN
23	V	17	GLN
23	V	31	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2686/2923 (91%)	624 (23%)	26 (0%)
2	Y	113/114 (99%)	16 (14%)	0
All	All	2799/3037 (92%)	640 (22%)	26 (0%)

5 of 640 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	2	A
1	X	9	U
1	X	15	G
1	X	33	U
1	X	34	U

5 of 26 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	1526	G

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Mol	Chain	Res	Type
1	X	1954	A
1	X	2806	U
1	X	1952	C
1	X	2234	C

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 466 ligands modelled in this entry, 422 are monoatomic - leaving 44 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
30	MPD	X	3004	-	7,7,7	0.30	0	9,10,10	0.27	0
30	MPD	X	3015	-	7,7,7	0.28	0	9,10,10	0.18	0
35	EOH	X	3440	-	2,2,2	0.57	0	1,1,1	0.68	0
35	EOH	X	3439	-	2,2,2	0.50	0	1,1,1	0.83	0
35	EOH	X	3436	-	2,2,2	0.56	0	1,1,1	0.63	0
33	EPE	X	3421	-	15,15,15	1.27	1 (6%)	19,20,20	0.22	0
30	MPD	X	3014	-	7,7,7	0.42	0	9,10,10	0.27	0
35	EOH	X	3442	-	2,2,2	0.59	0	1,1,1	0.56	0
34	SPD	X	3429	-	9,9,9	0.19	0	8,8,8	0.33	0
35	EOH	X	3435	-	2,2,2	0.56	0	1,1,1	0.62	0
34	SPD	X	3432	-	9,9,9	0.22	0	8,8,8	0.26	0
30	MPD	X	3012	-	7,7,7	0.33	0	9,10,10	0.25	0
34	SPD	X	3431	-	9,9,9	0.10	0	8,8,8	0.08	0
30	MPD	X	3011	-	7,7,7	0.58	0	9,10,10	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	EOH	X	3438	-	2,2,2	0.54	0	1,1,1	0.64	0
30	MPD	X	3007	-	7,7,7	0.46	0	9,10,10	0.22	0
30	MPD	X	3013	-	7,7,7	0.40	0	9,10,10	0.18	0
34	SPD	X	3425	-	9,9,9	0.18	0	8,8,8	0.24	0
34	SPD	X	3427	-	9,9,9	0.17	0	8,8,8	0.27	0
34	SPD	X	3433	-	9,9,9	0.13	0	8,8,8	0.18	0
29	3LK	X	3001	-	39,43,43	1.13	2 (5%)	53,67,67	1.87	7 (13%)
35	EOH	X	3443	-	2,2,2	0.56	0	1,1,1	0.62	0
35	EOH	X	3437	-	2,2,2	0.51	0	1,1,1	0.74	0
35	EOH	X	3441	-	2,2,2	0.51	0	1,1,1	0.75	0
35	EOH	W	101	-	2,2,2	0.50	0	1,1,1	0.64	0
33	EPE	X	3422	-	15,15,15	1.04	1 (6%)	19,20,20	0.46	0
30	MPD	X	3008	-	7,7,7	0.42	0	9,10,10	0.31	0
34	SPD	X	3428	-	9,9,9	0.17	0	8,8,8	0.19	0
34	SPD	X	3430	-	9,9,9	0.16	0	8,8,8	0.35	0
34	SPD	X	3426	-	9,9,9	0.16	0	8,8,8	0.12	0
34	SPD	C	302	-	9,9,9	0.22	0	8,8,8	0.21	0
33	EPE	X	3423	-	15,15,15	1.08	1 (6%)	19,20,20	0.82	1 (5%)
30	MPD	X	3010	-	7,7,7	0.29	0	9,10,10	0.16	0
30	MPD	X	3005	-	7,7,7	0.39	0	9,10,10	0.32	0
30	MPD	X	3003	-	7,7,7	0.35	0	9,10,10	0.24	0
33	EPE	X	3424	-	15,15,15	0.94	1 (6%)	19,20,20	0.16	0
30	MPD	X	3016	-	7,7,7	0.81	0	9,10,10	0.58	0
35	EOH	Y	208	-	2,2,2	0.54	0	1,1,1	0.61	0
35	EOH	W	102	-	2,2,2	0.53	0	1,1,1	0.67	0
34	SPD	X	3434	-	9,9,9	0.05	0	8,8,8	0.29	0
30	MPD	X	3002	-	7,7,7	0.32	0	9,10,10	0.58	0
35	EOH	K	201	-	2,2,2	0.54	0	1,1,1	0.60	0
30	MPD	X	3009	-	7,7,7	0.54	0	9,10,10	0.20	0
30	MPD	X	3006	-	7,7,7	0.57	0	9,10,10	0.32	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
30	MPD	X	3004	-	-	5/5/5/5	-
30	MPD	X	3015	-	-	5/5/5/5	-
33	EPE	X	3421	-	-	4/9/19/19	0/1/1/1
30	MPD	X	3014	-	-	4/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	SPD	X	3429	-	-	3/7/7/7	-
34	SPD	X	3432	-	-	3/7/7/7	-
30	MPD	X	3012	-	-	3/5/5/5	-
34	SPD	X	3431	-	-	1/7/7/7	-
30	MPD	X	3011	-	-	3/5/5/5	-
30	MPD	X	3007	-	-	2/5/5/5	-
30	MPD	X	3013	-	-	2/5/5/5	-
34	SPD	X	3425	-	-	2/7/7/7	-
34	SPD	X	3427	-	-	3/7/7/7	-
34	SPD	X	3433	-	-	2/7/7/7	-
29	3LK	X	3001	-	-	5/22/95/95	0/4/4/4
33	EPE	X	3422	-	-	1/9/19/19	0/1/1/1
30	MPD	X	3008	-	-	2/5/5/5	-
34	SPD	X	3428	-	-	4/7/7/7	-
34	SPD	X	3430	-	-	3/7/7/7	-
34	SPD	X	3426	-	-	3/7/7/7	-
34	SPD	C	302	-	-	0/7/7/7	-
33	EPE	X	3423	-	-	3/9/19/19	0/1/1/1
30	MPD	X	3010	-	-	0/5/5/5	-
30	MPD	X	3005	-	-	2/5/5/5	-
30	MPD	X	3003	-	-	2/5/5/5	-
33	EPE	X	3424	-	-	0/9/19/19	0/1/1/1
30	MPD	X	3016	-	-	0/5/5/5	-
34	SPD	X	3434	-	-	2/7/7/7	-
30	MPD	X	3002	-	-	2/5/5/5	-
30	MPD	X	3009	-	-	0/5/5/5	-
30	MPD	X	3006	-	-	2/5/5/5	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	X	3001	3LK	C20-C19	-5.87	1.27	1.51
33	X	3421	EPE	C10-S	-4.87	1.70	1.77
33	X	3423	EPE	C10-S	-4.09	1.71	1.77
33	X	3422	EPE	C10-S	-3.90	1.72	1.77
33	X	3424	EPE	C10-S	-3.63	1.72	1.77

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	3001	3LK	C20-C19-C12	7.61	126.10	116.24
29	X	3001	3LK	C15-C5-C14	-5.94	102.74	108.81
29	X	3001	3LK	C13-C14-C5	-5.17	110.73	116.28
29	X	3001	3LK	O3-C14-C5	4.28	112.98	106.32
29	X	3001	3LK	C22-S-C23	-2.83	96.71	101.75

There are no chirality outliers.

5 of 73 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	X	3001	3LK	C13-C12-C19-C20
29	X	3001	3LK	C27-C23-S-C22
30	X	3002	MPD	C1-C2-C3-C4
30	X	3004	MPD	C2-C3-C4-O4
30	X	3004	MPD	C2-C3-C4-C5

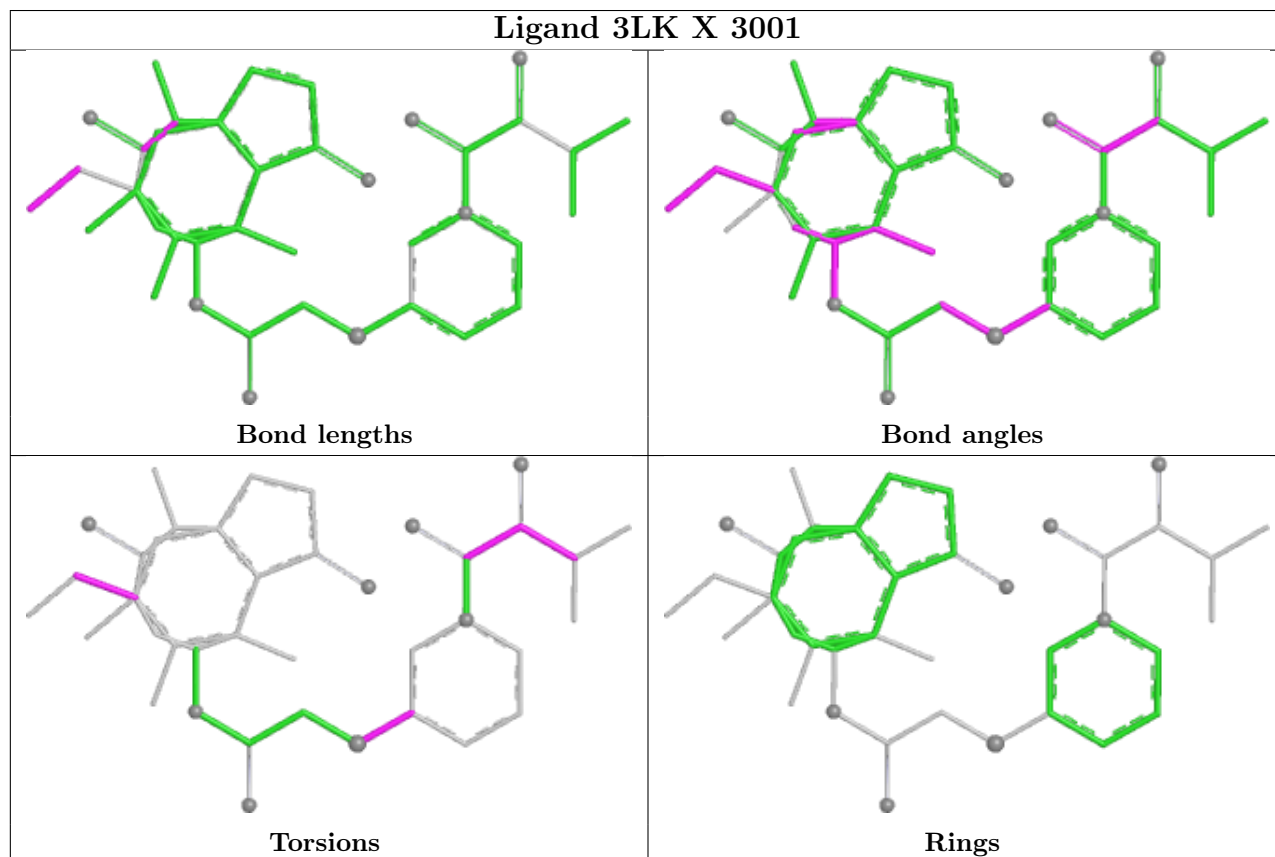
There are no ring outliers.

19 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	X	3004	MPD	2	0
30	X	3015	MPD	3	0
33	X	3421	EPE	4	0
30	X	3014	MPD	1	0
34	X	3429	SPD	1	0
34	X	3432	SPD	1	0
34	X	3431	SPD	1	0
29	X	3001	3LK	8	0
33	X	3422	EPE	1	0
30	X	3008	MPD	1	0
34	X	3428	SPD	1	0
34	X	3426	SPD	2	0
34	C	302	SPD	1	0
33	X	3423	EPE	2	0
30	X	3005	MPD	4	0
33	X	3424	EPE	3	0
30	X	3016	MPD	4	0
34	X	3434	SPD	6	0
30	X	3002	MPD	1	0

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.



5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	X	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	X	2123:A	O3'	2124:U	P	4.01

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	X	2707/2923 (92%)	-0.24	123 (4%) 38 24	26, 70, 166, 275	0
2	Y	114/114 (100%)	-0.33	1 (0%) 81 62	51, 84, 141, 183	0
3	A	271/277 (97%)	1.00	55 (20%) 3 3	54, 100, 155, 195	0
4	B	215/220 (97%)	0.60	31 (14%) 6 6	34, 49, 101, 134	0
5	C	199/207 (96%)	0.32	15 (7%) 20 15	37, 60, 111, 160	0
6	D	139/179 (77%)	1.18	33 (23%) 2 3	92, 142, 196, 234	0
7	E	156/178 (87%)	0.95	30 (19%) 3 3	58, 109, 176, 210	0
8	G	145/145 (100%)	0.78	24 (16%) 4 5	37, 49, 76, 133	0
9	H	122/122 (100%)	0.28	12 (9%) 13 11	58, 69, 108, 134	0
10	I	131/146 (89%)	1.31	43 (32%) 1 1	19, 73, 143, 206	0
11	J	136/144 (94%)	0.75	22 (16%) 4 5	41, 65, 127, 172	0
12	K	119/122 (97%)	0.47	12 (10%) 12 10	34, 57, 127, 151	0
13	L	110/119 (92%)	0.93	18 (16%) 4 5	56, 87, 131, 174	0
14	M	109/116 (93%)	0.39	15 (13%) 6 6	47, 64, 135, 177	0
15	N	116/118 (98%)	0.39	10 (8%) 16 13	24, 39, 87, 129	0
16	O	101/102 (99%)	-0.14	1 (0%) 79 60	23, 56, 101, 154	0
17	P	109/117 (93%)	0.26	9 (8%) 17 14	37, 49, 97, 134	0
18	Q	89/91 (97%)	1.38	22 (24%) 2 3	37, 88, 133, 162	0
19	R	100/105 (95%)	1.22	23 (23%) 2 3	35, 90, 171, 210	0
20	S	157/217 (72%)	0.16	7 (4%) 38 24	46, 78, 157, 244	0
21	T	75/94 (79%)	0.78	13 (17%) 4 4	33, 58, 109, 130	0
22	U	44/62 (70%)	3.43	35 (79%) 0 0	78, 120, 166, 218	0
23	V	65/69 (94%)	1.01	12 (18%) 3 4	79, 108, 170, 237	0
24	W	57/59 (96%)	0.23	7 (12%) 8 8	35, 45, 87, 95	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Z	44/58 (75%)	0.58	4 (9%) 15 12	28, 51, 130, 153	0
26	2	44/45 (97%)	0.22	0 100 100	54, 63, 85, 112	0
27	3	60/66 (90%)	1.00	8 (13%) 7 7	31, 53, 78, 94	0
28	4	37/37 (100%)	2.38	20 (54%) 0 0	56, 78, 106, 118	0
All	All	5771/6252 (92%)	0.26	605 (10%) 11 10	19, 71, 158, 275	0

The worst 5 of 605 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
28	4	28	GLU	10.3
9	H	36	GLY	9.6
7	E	166	GLY	9.5
1	X	2240	U	9.5
7	E	169	VAL	9.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 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	MPD	X	3006	8/8	0.25	0.39	110,110,110,110	0
31	MG	X	3092	1/1	0.26	0.33	66,66,66,66	0
30	MPD	X	3009	8/8	0.36	0.35	91,91,91,91	0
35	EOH	X	3442	3/3	0.36	0.42	68,68,68,68	0
35	EOH	X	3436	3/3	0.41	0.48	69,69,69,69	0
30	MPD	X	3007	8/8	0.42	0.34	87,87,87,87	0
31	MG	X	3123	1/1	0.45	0.33	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
31	MG	X	3112	1/1	0.46	0.13	23,23,23,23	1
32	MN	X	3218	1/1	0.49	0.18	170,170,170,170	0
30	MPD	X	3008	8/8	0.50	0.27	98,98,98,98	0
31	MG	X	3186	1/1	0.51	0.35	15,15,15,15	1
31	MG	X	3101	1/1	0.53	0.30	80,80,80,80	0
31	MG	X	3171	1/1	0.53	0.17	75,75,75,75	0
32	MN	X	3021	1/1	0.54	0.19	118,118,118,118	0
31	MG	X	3173	1/1	0.55	0.32	34,34,34,34	1
34	SPD	X	3432	10/10	0.57	0.35	63,63,63,63	0
34	SPD	X	3430	10/10	0.60	0.37	65,65,65,65	0
31	MG	X	3093	1/1	0.60	0.30	77,77,77,77	0
32	MN	X	3228	1/1	0.61	0.20	190,190,190,190	0
32	MN	X	3356	1/1	0.61	0.20	95,95,95,95	0
31	MG	X	3108	1/1	0.63	0.14	74,74,74,74	0
31	MG	X	3046	1/1	0.63	0.22	67,67,67,67	0
31	MG	X	3167	1/1	0.64	0.64	108,108,108,108	0
31	MG	X	3069	1/1	0.64	0.41	12,12,12,12	1
30	MPD	X	3003	8/8	0.65	0.66	82,82,82,82	0
32	MN	X	3098	1/1	0.65	0.15	143,143,143,143	0
31	MG	X	3412	1/1	0.65	0.22	73,73,73,73	0
32	MN	X	3249	1/1	0.67	0.12	149,149,149,149	0
31	MG	X	3177	1/1	0.67	0.37	64,64,64,64	0
31	MG	X	3185	1/1	0.68	0.36	74,74,74,74	0
34	SPD	X	3428	10/10	0.68	0.59	55,55,55,55	0
31	MG	X	3091	1/1	0.69	0.20	69,69,69,69	0
34	SPD	X	3431	10/10	0.69	0.37	56,56,56,56	10
32	MN	X	3361	1/1	0.69	0.27	148,148,148,148	0
32	MN	X	3383	1/1	0.69	0.14	156,156,156,156	0
31	MG	X	3411	1/1	0.69	0.29	78,78,78,78	0
32	MN	X	3367	1/1	0.70	0.27	128,128,128,128	0
32	MN	X	3184	1/1	0.70	0.39	139,139,139,139	0
35	EOH	X	3443	3/3	0.70	0.37	59,59,59,59	0
32	MN	X	3283	1/1	0.71	0.22	121,121,121,121	0
31	MG	X	3057	1/1	0.71	0.23	62,62,62,62	0
31	MG	X	3100	1/1	0.71	0.28	95,95,95,95	0
34	SPD	C	302	10/10	0.71	0.53	0,0,0,0	10
30	MPD	X	3014	8/8	0.71	0.28	105,105,105,105	0
32	MN	X	3032	1/1	0.71	0.07	170,170,170,170	0
32	MN	X	3036	1/1	0.71	0.16	177,177,177,177	0
31	MG	X	3124	1/1	0.73	0.18	50,50,50,50	0
32	MN	X	3354	1/1	0.73	0.17	114,114,114,114	0
31	MG	Y	204	1/1	0.74	0.16	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
31	MG	X	3089	1/1	0.74	0.49	91,91,91,91	0
32	MN	X	3231	1/1	0.74	0.16	166,166,166,166	0
32	MN	X	3085	1/1	0.75	0.16	185,185,185,185	0
30	MPD	X	3011	8/8	0.75	0.15	106,106,106,106	0
31	MG	Y	203	1/1	0.75	0.20	103,103,103,103	0
35	EOH	Y	208	3/3	0.75	0.63	89,89,89,89	0
31	MG	X	3129	1/1	0.76	0.17	54,54,54,54	0
32	MN	X	3023	1/1	0.76	0.30	193,193,193,193	0
32	MN	X	3152	1/1	0.76	0.12	136,136,136,136	0
35	EOH	X	3439	3/3	0.76	0.22	64,64,64,64	0
31	MG	X	3413	1/1	0.76	0.18	52,52,52,52	0
32	MN	X	3198	1/1	0.76	0.25	154,154,154,154	0
31	MG	E	201	1/1	0.76	0.16	45,45,45,45	0
35	EOH	X	3438	3/3	0.77	0.50	77,77,77,77	0
32	MN	X	3192	1/1	0.77	0.13	125,125,125,125	0
31	MG	X	3055	1/1	0.77	0.21	50,50,50,50	0
32	MN	X	3190	1/1	0.77	0.11	151,151,151,151	0
32	MN	X	3253	1/1	0.77	0.14	134,134,134,134	0
32	MN	X	3394	1/1	0.78	0.14	105,105,105,105	0
32	MN	X	3320	1/1	0.78	0.18	91,91,91,91	0
32	MN	X	3261	1/1	0.78	0.12	139,139,139,139	0
31	MG	G	201	1/1	0.78	0.17	49,49,49,49	0
34	SPD	X	3427	10/10	0.79	0.52	72,72,72,72	0
32	MN	X	3145	1/1	0.79	0.17	136,136,136,136	0
31	MG	X	3111	1/1	0.79	0.11	25,25,25,25	0
32	MN	X	3346	1/1	0.79	0.10	83,83,83,83	0
32	MN	X	3359	1/1	0.80	0.14	125,125,125,125	0
31	MG	X	3122	1/1	0.80	0.33	92,92,92,92	0
31	MG	X	3031	1/1	0.80	0.35	64,64,64,64	0
31	MG	X	3054	1/1	0.80	0.41	64,64,64,64	0
32	MN	X	3391	1/1	0.80	0.24	132,132,132,132	0
31	MG	X	3121	1/1	0.80	0.37	81,81,81,81	0
32	MN	R	201	1/1	0.80	0.12	118,118,118,118	0
33	EPE	X	3422	15/15	0.80	0.16	155,155,155,155	0
32	MN	X	3147	1/1	0.80	0.11	127,127,127,127	0
32	MN	X	3260	1/1	0.80	0.29	154,154,154,154	0
32	MN	X	3357	1/1	0.81	0.28	134,134,134,134	0
32	MN	X	3143	1/1	0.81	0.12	157,157,157,157	0
32	MN	X	3316	1/1	0.81	0.23	131,131,131,131	0
32	MN	X	3034	1/1	0.81	0.14	182,182,182,182	0
31	MG	B	301	1/1	0.81	0.16	23,23,23,23	0
32	MN	X	3025	1/1	0.81	0.15	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
31	MG	X	3028	1/1	0.81	0.52	66,66,66,66	0
31	MG	A	302	1/1	0.82	0.36	38,38,38,38	0
32	MN	X	3183	1/1	0.82	0.13	145,145,145,145	0
32	MN	X	3090	1/1	0.82	0.13	114,114,114,114	0
30	MPD	X	3002	8/8	0.82	0.28	56,56,56,56	0
32	MN	X	3131	1/1	0.82	0.23	134,134,134,134	0
31	MG	Y	201	1/1	0.82	0.16	83,83,83,83	0
31	MG	X	3051	1/1	0.82	0.31	64,64,64,64	0
31	MG	X	3056	1/1	0.82	0.29	68,68,68,68	0
35	EOH	K	201	3/3	0.82	0.18	17,17,17,17	0
32	MN	X	3358	1/1	0.83	0.20	122,122,122,122	0
32	MN	X	3075	1/1	0.83	0.11	136,136,136,136	0
33	EPE	X	3424	15/15	0.83	0.22	137,137,137,137	0
32	MN	X	3255	1/1	0.83	0.23	217,217,217,217	0
31	MG	X	3070	1/1	0.83	0.11	91,91,91,91	0
32	MN	X	3139	1/1	0.83	0.10	132,132,132,132	0
32	MN	X	3066	1/1	0.83	0.13	146,146,146,146	0
32	MN	X	3311	1/1	0.83	0.14	140,140,140,140	0
32	MN	X	3205	1/1	0.84	0.18	101,101,101,101	0
32	MN	X	3374	1/1	0.84	0.10	69,69,69,69	0
32	MN	X	3333	1/1	0.84	0.17	117,117,117,117	0
31	MG	X	3116	1/1	0.84	0.11	95,95,95,95	0
31	MG	O	201	1/1	0.84	0.33	30,30,30,30	0
35	EOH	X	3437	3/3	0.84	0.60	108,108,108,108	0
32	MN	X	3444	1/1	0.84	0.26	70,70,70,70	0
32	MN	X	3165	1/1	0.84	0.09	104,104,104,104	0
35	EOH	X	3441	3/3	0.84	0.46	82,82,82,82	0
32	MN	X	3292	1/1	0.84	0.13	90,90,90,90	0
32	MN	X	3065	1/1	0.84	0.31	67,67,67,67	1
32	MN	X	3315	1/1	0.84	0.23	143,143,143,143	0
32	MN	X	3203	1/1	0.84	0.10	96,96,96,96	0
31	MG	X	3102	1/1	0.85	0.08	33,33,33,33	0
31	MG	X	3119	1/1	0.85	0.37	87,87,87,87	0
32	MN	X	3363	1/1	0.85	0.15	130,130,130,130	0
33	EPE	X	3423	15/15	0.85	0.39	145,145,145,145	0
32	MN	X	3088	1/1	0.85	0.16	149,149,149,149	0
30	MPD	X	3016	8/8	0.85	0.34	32,32,32,32	0
31	MG	X	3182	1/1	0.85	0.15	66,66,66,66	0
32	MN	X	3202	1/1	0.85	0.23	151,151,151,151	0
31	MG	X	3115	1/1	0.85	0.12	58,58,58,58	0
32	MN	X	3399	1/1	0.85	0.18	130,130,130,130	0
35	EOH	W	101	3/3	0.85	0.19	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
30	MPD	X	3013	8/8	0.86	0.52	95,95,95,95	0
32	MN	X	3067	1/1	0.86	0.18	80,80,80,80	1
32	MN	X	3389	1/1	0.86	0.07	105,105,105,105	0
32	MN	X	3350	1/1	0.86	0.18	139,139,139,139	0
32	MN	X	3223	1/1	0.86	0.15	131,131,131,131	0
32	MN	X	3148	1/1	0.86	0.14	124,124,124,124	0
30	MPD	X	3004	8/8	0.86	0.42	101,101,101,101	0
32	MN	Y	206	1/1	0.86	0.14	87,87,87,87	0
32	MN	X	3300	1/1	0.86	0.12	107,107,107,107	0
32	MN	X	3243	1/1	0.86	0.08	73,73,73,73	0
31	MG	X	3120	1/1	0.86	0.23	66,66,66,66	0
32	MN	X	3362	1/1	0.86	0.20	99,99,99,99	0
31	MG	X	3168	1/1	0.86	0.23	57,57,57,57	0
32	MN	X	3254	1/1	0.86	0.12	106,106,106,106	0
32	MN	X	3195	1/1	0.87	0.17	129,129,129,129	0
32	MN	X	3241	1/1	0.87	0.09	85,85,85,85	0
32	MN	X	3063	1/1	0.87	0.21	78,78,78,78	0
32	MN	X	3142	1/1	0.87	0.26	166,166,166,166	0
32	MN	X	3180	1/1	0.87	0.24	139,139,139,139	0
31	MG	X	3211	1/1	0.87	0.32	44,44,44,44	0
33	EPE	X	3421	15/15	0.87	0.35	117,117,117,117	4
32	MN	X	3215	1/1	0.87	0.11	101,101,101,101	0
32	MN	X	3024	1/1	0.87	0.07	150,150,150,150	0
31	MG	X	3410	1/1	0.87	0.33	49,49,49,49	1
32	MN	X	3352	1/1	0.87	0.14	142,142,142,142	0
32	MN	X	3388	1/1	0.87	0.09	121,121,121,121	0
32	MN	X	3037	1/1	0.87	0.18	135,135,135,135	0
32	MN	X	3403	1/1	0.88	0.15	98,98,98,98	0
31	MG	X	3042	1/1	0.88	0.09	75,75,75,75	0
32	MN	X	3033	1/1	0.88	0.20	136,136,136,136	0
32	MN	X	3233	1/1	0.88	0.11	97,97,97,97	0
32	MN	X	3353	1/1	0.88	0.22	92,92,92,92	0
31	MG	X	3059	1/1	0.88	0.11	34,34,34,34	0
31	MG	X	3113	1/1	0.88	0.06	34,34,34,34	0
31	MG	X	3049	1/1	0.88	0.54	80,80,80,80	0
32	MN	X	3135	1/1	0.88	0.10	114,114,114,114	0
32	MN	X	3041	1/1	0.88	0.34	185,185,185,185	0
32	MN	X	3196	1/1	0.88	0.10	88,88,88,88	0
31	MG	X	3109	1/1	0.88	0.09	46,46,46,46	0
31	MG	X	3418	1/1	0.88	0.22	51,51,51,51	0
32	MN	X	3144	1/1	0.88	0.13	116,116,116,116	0
31	MG	X	3127	1/1	0.88	0.05	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
32	MN	X	3375	1/1	0.88	0.19	129,129,129,129	0
32	MN	X	3378	1/1	0.88	0.27	141,141,141,141	0
32	MN	X	3212	1/1	0.88	0.13	106,106,106,106	0
31	MG	X	3128	1/1	0.88	0.16	61,61,61,61	0
31	MG	X	3110	1/1	0.88	0.07	51,51,51,51	0
32	MN	X	3220	1/1	0.88	0.17	133,133,133,133	0
32	MN	X	3222	1/1	0.88	0.24	150,150,150,150	0
32	MN	X	3397	1/1	0.88	0.10	106,106,106,106	0
32	MN	X	3079	1/1	0.88	0.19	145,145,145,145	0
35	EOH	W	102	3/3	0.88	0.34	66,66,66,66	0
32	MN	X	3244	1/1	0.89	0.14	138,138,138,138	0
34	SPD	X	3425	10/10	0.89	0.29	101,101,101,101	0
32	MN	X	3159	1/1	0.89	0.10	137,137,137,137	0
32	MN	X	3160	1/1	0.89	0.08	126,126,126,126	0
31	MG	B	302	1/1	0.89	0.20	34,34,34,34	0
32	MN	X	3179	1/1	0.89	0.14	140,140,140,140	0
32	MN	X	3137	1/1	0.89	0.12	110,110,110,110	0
31	MG	X	3106	1/1	0.89	0.31	28,28,28,28	1
32	MN	X	3396	1/1	0.89	0.06	109,109,109,109	0
30	MPD	X	3012	8/8	0.89	0.55	87,87,87,87	0
31	MG	X	3052	1/1	0.89	0.17	26,26,26,26	0
31	MG	X	3226	1/1	0.89	0.20	57,57,57,57	0
32	MN	X	3040	1/1	0.89	0.20	157,157,157,157	0
32	MN	Y	202	1/1	0.89	0.05	124,124,124,124	0
31	MG	X	3030	1/1	0.89	0.22	59,59,59,59	0
31	MG	X	3050	1/1	0.89	0.29	83,83,83,83	0
32	MN	X	3364	1/1	0.89	0.11	78,78,78,78	0
31	MG	X	3105	1/1	0.89	0.22	56,56,56,56	0
32	MN	X	3323	1/1	0.89	0.13	71,71,71,71	0
32	MN	X	3157	1/1	0.90	0.06	103,103,103,103	0
32	MN	X	3197	1/1	0.90	0.24	111,111,111,111	0
31	MG	X	3130	1/1	0.90	0.21	65,65,65,65	0
32	MN	X	3199	1/1	0.90	0.11	130,130,130,130	0
32	MN	X	3018	1/1	0.90	0.09	116,116,116,116	0
32	MN	X	3355	1/1	0.90	0.08	115,115,115,115	0
32	MN	X	3163	1/1	0.90	0.14	143,143,143,143	0
32	MN	X	3084	1/1	0.90	0.25	148,148,148,148	0
32	MN	X	3209	1/1	0.90	0.10	157,157,157,157	0
32	MN	X	3256	1/1	0.90	0.13	133,133,133,133	0
32	MN	X	3020	1/1	0.90	0.11	120,120,120,120	0
32	MN	X	3086	1/1	0.90	0.05	122,122,122,122	0
32	MN	X	3264	1/1	0.90	0.20	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
30	MPD	X	3005	8/8	0.90	0.24	99,99,99,99	0
32	MN	X	3288	1/1	0.90	0.16	87,87,87,87	0
32	MN	X	3372	1/1	0.90	0.19	101,101,101,101	0
34	SPD	X	3433	10/10	0.90	0.41	97,97,97,97	0
34	SPD	X	3434	10/10	0.90	0.47	91,91,91,91	0
32	MN	X	3373	1/1	0.90	0.08	139,139,139,139	0
32	MN	X	3219	1/1	0.90	0.10	119,119,119,119	0
31	MG	X	3103	1/1	0.90	0.10	78,78,78,78	0
31	MG	X	3117	1/1	0.90	0.27	34,34,34,34	0
32	MN	X	3379	1/1	0.90	0.18	98,98,98,98	0
32	MN	X	3314	1/1	0.90	0.29	116,116,116,116	0
32	MN	X	3073	1/1	0.90	0.08	140,140,140,140	0
32	MN	X	3193	1/1	0.90	0.11	107,107,107,107	0
32	MN	X	3317	1/1	0.90	0.14	112,112,112,112	0
32	MN	X	3229	1/1	0.90	0.11	76,76,76,76	0
32	MN	X	3230	1/1	0.90	0.12	118,118,118,118	0
32	MN	X	3133	1/1	0.90	0.14	139,139,139,139	0
32	MN	X	3080	1/1	0.91	0.09	111,111,111,111	0
31	MG	X	3408	1/1	0.91	0.11	62,62,62,62	0
32	MN	X	3252	1/1	0.91	0.08	127,127,127,127	0
32	MN	X	3404	1/1	0.91	0.11	116,116,116,116	0
31	MG	X	3409	1/1	0.91	0.32	35,35,35,35	1
32	MN	X	3445	1/1	0.91	0.15	108,108,108,108	0
32	MN	X	3156	1/1	0.91	0.09	127,127,127,127	0
31	MG	X	3176	1/1	0.91	0.05	39,39,39,39	0
32	MN	X	3035	1/1	0.91	0.11	110,110,110,110	0
31	MG	X	3043	1/1	0.91	0.22	75,75,75,75	0
32	MN	X	3162	1/1	0.91	0.10	130,130,130,130	0
31	MG	X	3118	1/1	0.91	0.23	59,59,59,59	0
32	MN	X	3360	1/1	0.91	0.17	122,122,122,122	0
32	MN	X	3269	1/1	0.91	0.10	71,71,71,71	0
34	SPD	X	3426	10/10	0.91	0.14	71,71,71,71	0
32	MN	X	3276	1/1	0.91	0.07	75,75,75,75	0
31	MG	X	3044	1/1	0.91	0.06	27,27,27,27	0
34	SPD	X	3429	10/10	0.91	0.13	61,61,61,61	0
32	MN	X	3166	1/1	0.91	0.18	115,115,115,115	0
31	MG	X	3414	1/1	0.91	0.20	64,64,64,64	0
32	MN	X	3019	1/1	0.91	0.20	148,148,148,148	0
32	MN	X	3301	1/1	0.91	0.13	98,98,98,98	0
31	MG	X	3417	1/1	0.91	0.11	45,45,45,45	0
31	MG	X	3126	1/1	0.91	0.17	51,51,51,51	0
32	MN	X	3141	1/1	0.91	0.09	127,127,127,127	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
32	MN	X	3191	1/1	0.91	0.07	75,75,75,75	0
32	MN	X	3380	1/1	0.91	0.19	128,128,128,128	0
32	MN	X	3381	1/1	0.91	0.07	102,102,102,102	0
32	MN	X	3022	1/1	0.91	0.19	133,133,133,133	0
32	MN	X	3385	1/1	0.91	0.11	108,108,108,108	0
31	MG	X	3187	1/1	0.91	0.09	52,52,52,52	0
32	MN	X	3321	1/1	0.91	0.19	116,116,116,116	0
30	MPD	X	3010	8/8	0.91	0.22	129,129,129,129	0
31	MG	X	3107	1/1	0.91	0.11	58,58,58,58	0
32	MN	X	3335	1/1	0.91	0.27	67,67,67,67	0
32	MN	X	3216	1/1	0.92	0.19	128,128,128,128	0
31	MG	Y	207	1/1	0.92	0.20	20,20,20,20	1
32	MN	X	3262	1/1	0.92	0.11	59,59,59,59	0
32	MN	X	3263	1/1	0.92	0.17	71,71,71,71	0
31	MG	X	3047	1/1	0.92	0.19	75,75,75,75	0
32	MN	X	3268	1/1	0.92	0.14	73,73,73,73	0
32	MN	X	3134	1/1	0.92	0.07	122,122,122,122	0
31	MG	X	3071	1/1	0.92	0.29	100,100,100,100	0
32	MN	X	3368	1/1	0.92	0.10	101,101,101,101	0
32	MN	X	3078	1/1	0.92	0.07	130,130,130,130	0
32	MN	X	3337	1/1	0.92	0.11	70,70,70,70	0
32	MN	X	3038	1/1	0.92	0.13	127,127,127,127	0
32	MN	Y	205	1/1	0.92	0.07	103,103,103,103	0
32	MN	X	3194	1/1	0.92	0.25	177,177,177,177	0
32	MN	A	301	1/1	0.92	0.11	119,119,119,119	0
32	MN	X	3296	1/1	0.92	0.07	78,78,78,78	0
32	MN	X	3096	1/1	0.92	0.07	144,144,144,144	0
32	MN	X	3039	1/1	0.92	0.05	153,153,153,153	0
32	MN	X	3302	1/1	0.92	0.14	87,87,87,87	0
32	MN	X	3308	1/1	0.92	0.17	103,103,103,103	0
32	MN	X	3259	1/1	0.92	0.20	162,162,162,162	0
32	MN	X	3258	1/1	0.93	0.15	132,132,132,132	0
32	MN	X	3339	1/1	0.93	0.17	67,67,67,67	0
32	MN	X	3217	1/1	0.93	0.11	92,92,92,92	0
32	MN	X	3097	1/1	0.93	0.10	108,108,108,108	0
31	MG	X	3114	1/1	0.93	0.11	37,37,37,37	0
31	MG	X	3017	1/1	0.93	0.18	53,53,53,53	0
32	MN	X	3305	1/1	0.93	0.19	80,80,80,80	0
32	MN	X	3306	1/1	0.93	0.22	69,69,69,69	0
32	MN	X	3307	1/1	0.93	0.08	78,78,78,78	0
32	MN	X	3246	1/1	0.93	0.22	86,86,86,86	0
32	MN	X	3392	1/1	0.93	0.17	137,137,137,137	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MN	X	3393	1/1	0.93	0.15	80,80,80,80	0
32	MN	X	3208	1/1	0.93	0.17	104,104,104,104	0
32	MN	X	3313	1/1	0.93	0.10	88,88,88,88	0
32	MN	X	3266	1/1	0.93	0.19	83,83,83,83	0
31	MG	X	3026	1/1	0.93	0.23	50,50,50,50	0
32	MN	X	3400	1/1	0.93	0.06	106,106,106,106	0
32	MN	X	3210	1/1	0.93	0.11	140,140,140,140	0
32	MN	X	3275	1/1	0.93	0.08	77,77,77,77	0
32	MN	X	3164	1/1	0.93	0.07	104,104,104,104	0
32	MN	X	3281	1/1	0.93	0.10	61,61,61,61	0
32	MN	X	3282	1/1	0.93	0.22	105,105,105,105	0
32	MN	X	3370	1/1	0.93	0.15	86,86,86,86	0
32	MN	X	3327	1/1	0.93	0.12	99,99,99,99	0
31	MG	X	3094	1/1	0.93	0.16	58,58,58,58	0
31	MG	X	3058	1/1	0.93	0.31	95,95,95,95	0
31	MG	X	3169	1/1	0.94	0.10	32,32,32,32	0
32	MN	X	3242	1/1	0.94	0.07	100,100,100,100	0
32	MN	X	3270	1/1	0.94	0.18	60,60,60,60	0
32	MN	X	3319	1/1	0.94	0.14	101,101,101,101	0
32	MN	X	3369	1/1	0.94	0.05	85,85,85,85	0
31	MG	X	3029	1/1	0.94	0.24	55,55,55,55	0
31	MG	X	3172	1/1	0.94	0.17	36,36,36,36	0
32	MN	X	3158	1/1	0.94	0.07	82,82,82,82	0
32	MN	X	3138	1/1	0.94	0.10	93,93,93,93	0
32	MN	X	3331	1/1	0.94	0.07	94,94,94,94	0
32	MN	X	3376	1/1	0.94	0.09	57,57,57,57	0
32	MN	X	3087	1/1	0.94	0.07	120,120,120,120	0
32	MN	X	3285	1/1	0.94	0.18	99,99,99,99	0
32	MN	X	3161	1/1	0.94	0.08	70,70,70,70	0
31	MG	X	3060	1/1	0.94	0.26	42,42,42,42	0
32	MN	X	3382	1/1	0.94	0.18	140,140,140,140	0
32	MN	X	3343	1/1	0.94	0.20	69,69,69,69	0
31	MG	X	3174	1/1	0.94	0.10	55,55,55,55	0
32	MN	X	3297	1/1	0.94	0.09	52,52,52,52	0
32	MN	X	3077	1/1	0.94	0.09	111,111,111,111	0
32	MN	X	3257	1/1	0.94	0.09	110,110,110,110	0
32	MN	X	3221	1/1	0.94	0.14	73,73,73,73	0
35	EOH	X	3435	3/3	0.94	0.51	62,62,62,62	0
32	MN	X	3304	1/1	0.94	0.08	81,81,81,81	0
31	MG	C	301	1/1	0.94	0.12	28,28,28,28	0
32	MN	X	3395	1/1	0.94	0.13	117,117,117,117	0
32	MN	X	3062	1/1	0.94	0.13	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MN	X	3201	1/1	0.94	0.04	85,85,85,85	0
31	MG	X	3104	1/1	0.94	0.06	42,42,42,42	0
32	MN	X	3082	1/1	0.94	0.07	48,48,48,48	0
32	MN	X	3204	1/1	0.94	0.05	78,78,78,78	0
32	MN	X	3181	1/1	0.94	0.07	91,91,91,91	0
32	MN	X	3405	1/1	0.94	0.06	84,84,84,84	0
32	MN	X	3406	1/1	0.94	0.13	87,87,87,87	0
31	MG	X	3175	1/1	0.95	0.13	17,17,17,17	0
32	MN	X	3206	1/1	0.95	0.10	111,111,111,111	0
32	MN	X	3207	1/1	0.95	0.05	94,94,94,94	0
31	MG	X	3099	1/1	0.95	0.04	59,59,59,59	0
32	MN	X	3365	1/1	0.95	0.06	69,69,69,69	0
31	MG	X	3027	1/1	0.95	0.22	38,38,38,38	0
31	MG	X	3407	1/1	0.95	0.04	31,31,31,31	0
32	MN	X	3279	1/1	0.95	0.06	78,78,78,78	0
32	MN	X	3341	1/1	0.95	0.23	33,33,33,33	0
32	MN	X	3371	1/1	0.95	0.18	109,109,109,109	0
31	MG	X	3415	1/1	0.95	0.05	38,38,38,38	0
32	MN	X	3309	1/1	0.95	0.13	77,77,77,77	0
31	MG	X	3125	1/1	0.95	0.15	46,46,46,46	0
32	MN	X	3351	1/1	0.95	0.11	117,117,117,117	0
32	MN	X	3234	1/1	0.95	0.09	70,70,70,70	0
30	MPD	X	3015	8/8	0.95	0.38	72,72,72,72	0
32	MN	X	3286	1/1	0.95	0.18	50,50,50,50	0
32	MN	X	3189	1/1	0.95	0.08	138,138,138,138	0
31	MG	X	3419	1/1	0.95	0.32	57,57,57,57	0
31	MG	X	3045	1/1	0.95	0.14	65,65,65,65	0
32	MN	X	3150	1/1	0.95	0.09	128,128,128,128	0
32	MN	X	3384	1/1	0.95	0.06	75,75,75,75	0
32	MN	X	3298	1/1	0.95	0.06	66,66,66,66	0
32	MN	X	3322	1/1	0.95	0.06	52,52,52,52	0
32	MN	X	3245	1/1	0.96	0.04	86,86,86,86	0
32	MN	X	3132	1/1	0.96	0.10	112,112,112,112	0
32	MN	X	3247	1/1	0.96	0.16	48,48,48,48	0
32	MN	X	3083	1/1	0.96	0.16	44,44,44,44	0
32	MN	X	3251	1/1	0.96	0.09	131,131,131,131	0
32	MN	X	3284	1/1	0.96	0.09	58,58,58,58	0
32	MN	X	3178	1/1	0.96	0.12	88,88,88,88	0
32	MN	X	3200	1/1	0.96	0.07	77,77,77,77	0
32	MN	X	3325	1/1	0.96	0.09	62,62,62,62	0
32	MN	X	3149	1/1	0.96	0.08	117,117,117,117	0
32	MN	X	3289	1/1	0.96	0.09	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
32	MN	X	3291	1/1	0.96	0.12	90,90,90,90	0
31	MG	X	3227	1/1	0.96	0.13	35,35,35,35	0
32	MN	X	3074	1/1	0.96	0.07	95,95,95,95	0
32	MN	X	3225	1/1	0.96	0.12	103,103,103,103	0
32	MN	X	3340	1/1	0.96	0.08	23,23,23,23	0
32	MN	X	3155	1/1	0.96	0.10	89,89,89,89	0
32	MN	X	3299	1/1	0.96	0.07	69,69,69,69	0
32	MN	X	3345	1/1	0.96	0.18	54,54,54,54	0
31	MG	X	3420	1/1	0.96	0.15	30,30,30,30	0
32	MN	X	3347	1/1	0.96	0.06	106,106,106,106	0
32	MN	X	3349	1/1	0.96	0.18	99,99,99,99	0
32	MN	X	3386	1/1	0.96	0.12	65,65,65,65	0
32	MN	X	3076	1/1	0.96	0.08	144,144,144,144	0
31	MG	X	3188	1/1	0.96	0.06	41,41,41,41	0
32	MN	X	3232	1/1	0.96	0.10	84,84,84,84	0
32	MN	X	3140	1/1	0.96	0.04	82,82,82,82	0
32	MN	X	3064	1/1	0.96	0.07	96,96,96,96	0
32	MN	X	3235	1/1	0.96	0.05	95,95,95,95	0
31	MG	X	3416	1/1	0.96	0.18	16,16,16,16	0
31	MG	X	3170	1/1	0.96	0.06	60,60,60,60	0
32	MN	X	3081	1/1	0.96	0.17	32,32,32,32	0
32	MN	X	3398	1/1	0.96	0.09	88,88,88,88	0
32	MN	X	3312	1/1	0.96	0.10	50,50,50,50	0
32	MN	X	3272	1/1	0.96	0.16	43,43,43,43	0
32	MN	X	3401	1/1	0.96	0.07	67,67,67,67	0
29	3LK	X	3001	40/40	0.96	0.12	31,31,31,31	0
32	MN	X	3267	1/1	0.97	0.13	74,74,74,74	0
32	MN	X	3336	1/1	0.97	0.12	48,48,48,48	0
31	MG	X	3053	1/1	0.97	0.10	53,53,53,53	0
32	MN	X	3402	1/1	0.97	0.08	67,67,67,67	0
32	MN	X	3338	1/1	0.97	0.17	67,67,67,67	0
32	MN	X	3248	1/1	0.97	0.27	71,71,71,71	0
32	MN	X	3236	1/1	0.97	0.16	85,85,85,85	0
32	MN	X	3303	1/1	0.97	0.17	118,118,118,118	0
32	MN	X	3213	1/1	0.97	0.07	72,72,72,72	0
32	MN	X	3274	1/1	0.97	0.12	37,37,37,37	0
32	MN	X	3136	1/1	0.97	0.04	84,84,84,84	0
32	MN	X	3146	1/1	0.97	0.14	88,88,88,88	0
32	MN	X	3390	1/1	0.97	0.09	97,97,97,97	0
32	MN	X	3294	1/1	0.97	0.07	47,47,47,47	0
32	MN	X	3151	1/1	0.97	0.09	69,69,69,69	0
32	MN	X	3326	1/1	0.97	0.09	42,42,42,42	0

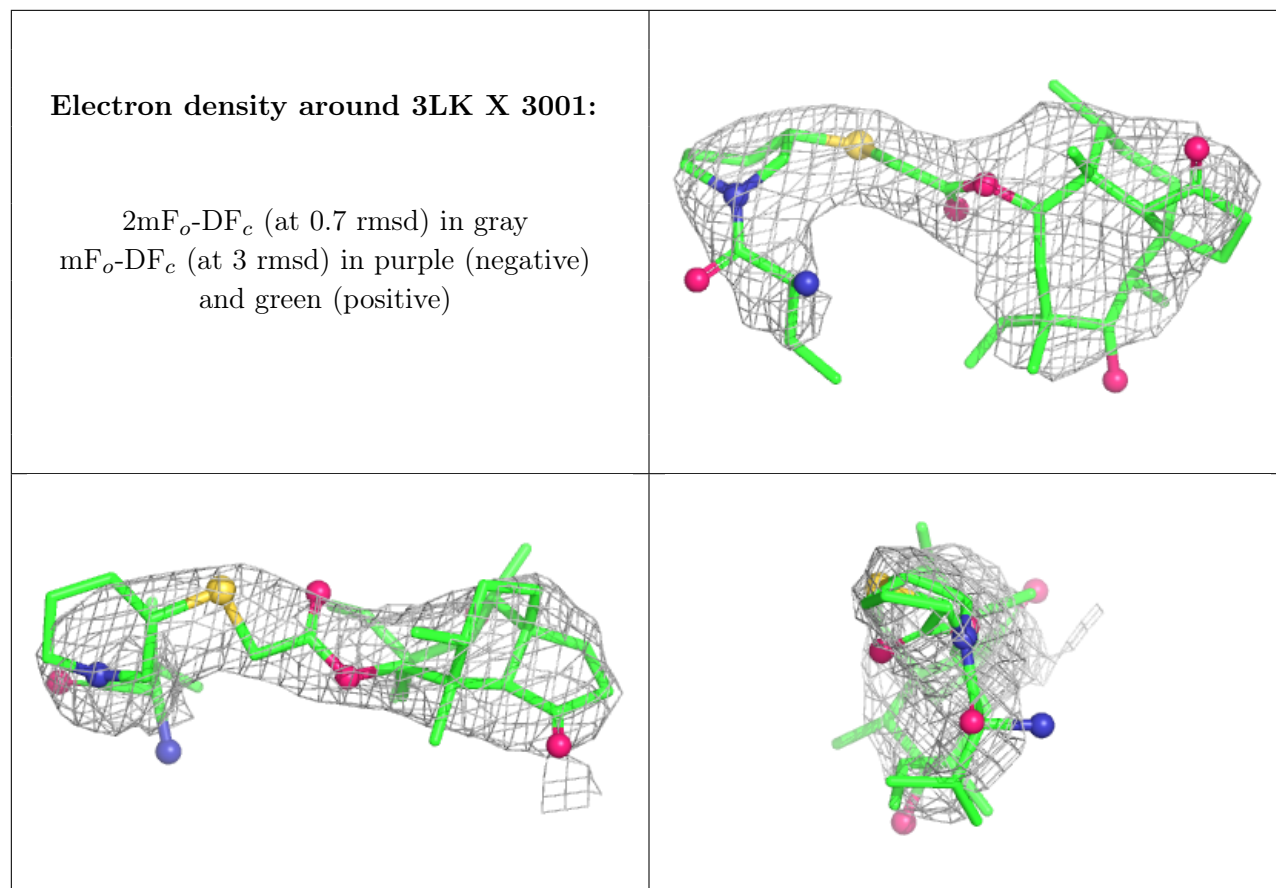
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MN	X	3310	1/1	0.97	0.19	97,97,97,97	0
32	MN	X	3329	1/1	0.97	0.14	53,53,53,53	0
32	MN	X	3224	1/1	0.97	0.08	104,104,104,104	0
32	MN	X	3332	1/1	0.97	0.19	109,109,109,109	0
32	MN	X	3061	1/1	0.97	0.18	68,68,68,68	0
32	MN	X	3344	1/1	0.98	0.12	46,46,46,46	0
32	MN	X	3273	1/1	0.98	0.08	35,35,35,35	0
32	MN	X	3240	1/1	0.98	0.06	73,73,73,73	0
32	MN	X	3324	1/1	0.98	0.05	47,47,47,47	0
32	MN	X	3290	1/1	0.98	0.08	66,66,66,66	0
31	MG	X	3048	1/1	0.98	0.20	49,49,49,49	0
32	MN	X	3265	1/1	0.98	0.08	60,60,60,60	0
32	MN	X	3328	1/1	0.98	0.07	48,48,48,48	0
32	MN	X	3277	1/1	0.98	0.04	35,35,35,35	0
32	MN	X	3377	1/1	0.98	0.11	55,55,55,55	0
32	MN	X	3330	1/1	0.98	0.06	55,55,55,55	0
32	MN	X	3295	1/1	0.98	0.04	55,55,55,55	0
32	MN	X	3278	1/1	0.98	0.04	55,55,55,55	0
32	MN	X	3068	1/1	0.98	0.10	34,34,34,34	0
32	MN	X	3334	1/1	0.98	0.14	48,48,48,48	0
32	MN	X	3280	1/1	0.98	0.04	50,50,50,50	0
32	MN	X	3250	1/1	0.98	0.03	66,66,66,66	0
35	EOH	X	3440	3/3	0.98	0.19	53,53,53,53	0
32	MN	X	3072	1/1	0.98	0.11	38,38,38,38	0
32	MN	X	3214	1/1	0.98	0.06	74,74,74,74	0
32	MN	X	3318	1/1	0.98	0.07	57,57,57,57	0
32	MN	X	3237	1/1	0.98	0.06	66,66,66,66	0
32	MN	X	3271	1/1	0.98	0.14	60,60,60,60	0
32	MN	X	3366	1/1	0.98	0.04	71,71,71,71	0
32	MN	X	3238	1/1	0.98	0.13	70,70,70,70	0
32	MN	X	3287	1/1	0.99	0.11	57,57,57,57	0
32	MN	X	3348	1/1	0.99	0.08	32,32,32,32	0
32	MN	X	3293	1/1	0.99	0.07	29,29,29,29	0
32	MN	X	3342	1/1	0.99	0.21	49,49,49,49	0
32	MN	X	3239	1/1	0.99	0.08	55,55,55,55	0
32	MN	X	3154	1/1	0.99	0.04	75,75,75,75	0
31	MG	X	3095	1/1	0.99	0.13	46,46,46,46	0
32	MN	X	3153	1/1	0.99	0.02	66,66,66,66	0
32	MN	X	3387	1/1	0.99	0.03	59,59,59,59	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.



6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.