wwPDB X-ray Structure Validation Summary Report (i)

Jan 4, 2024 – 01:39 am GMT

PDB ID	:	4WFB
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 (i) 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 (i)) were used in the production of this report:

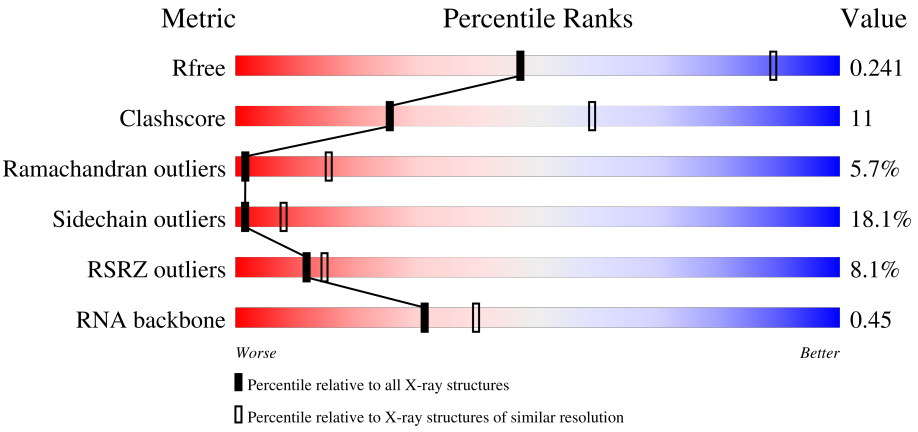
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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}	130704	1278 (3.50-3.38)
Clashscore	141614	1361 (3.50-3.38)
Ramachandran outliers	138981	1327 (3.50-3.38)
Sidechain outliers	138945	1328 (3.50-3.38)
RSRZ outliers	127900	1192 (3.50-3.38)
RNA backbone	3102	1024 (3.92-2.96)

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 <=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	2% 48% 34% 10% • 7%
2	Y	114	2% 41% 52% 6% •
3	A	277	16% 64% 27% 6% •

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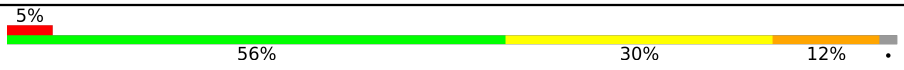
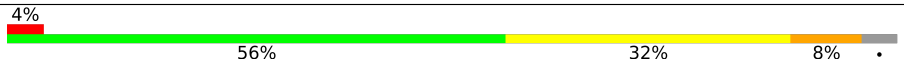
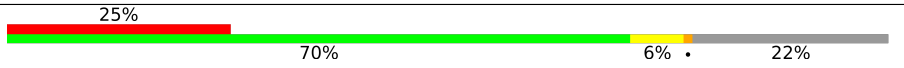
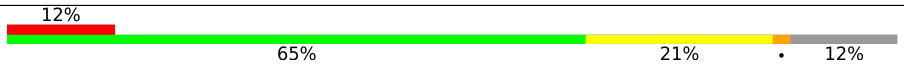
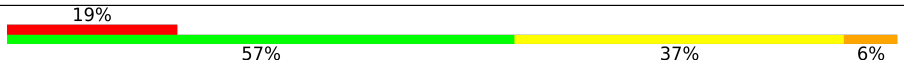
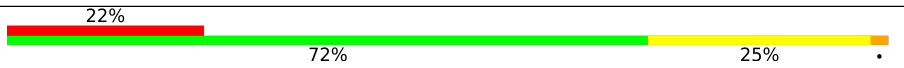
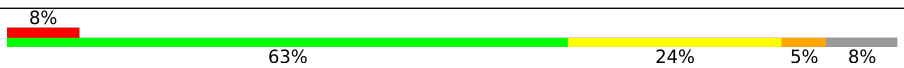
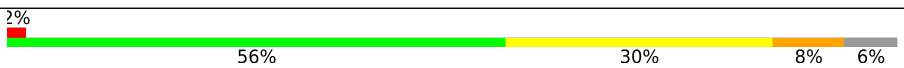
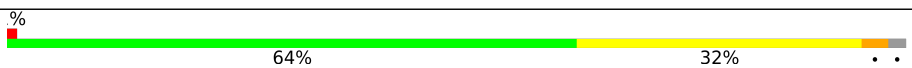
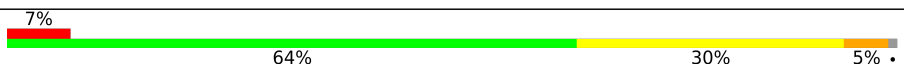
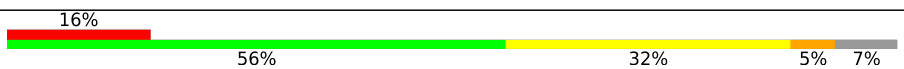
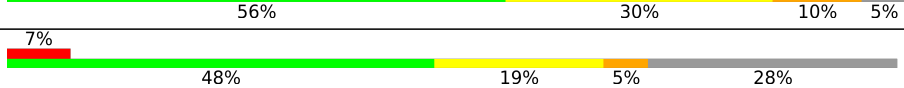
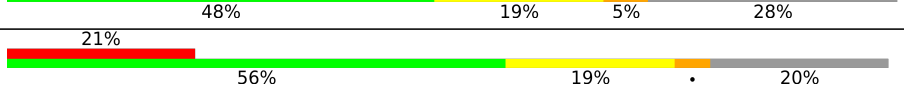
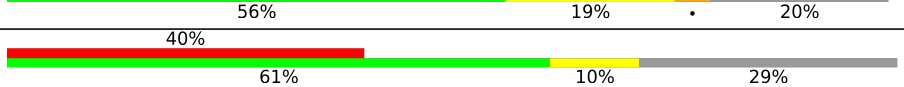
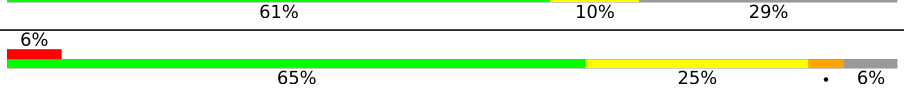
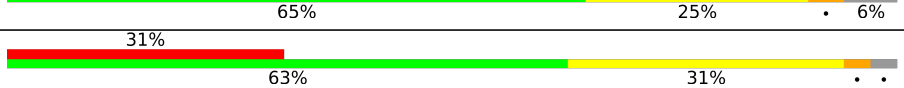
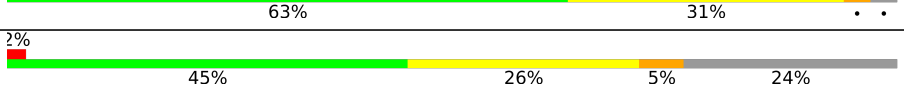
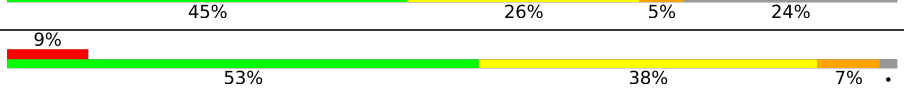
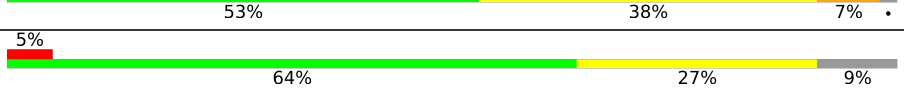
Mol	Chain	Length	Quality of chain
4	B	220	
5	C	207	
6	D	179	
7	E	178	
8	G	145	
9	H	122	
10	I	146	
11	J	144	
12	K	122	
13	L	119	
14	M	116	
15	N	118	
16	O	102	
17	P	117	
18	Q	91	
19	R	105	
20	S	217	
21	T	94	
22	U	62	
23	V	69	
24	W	59	
25	Z	58	
26	2	45	
27	3	66	
28	4	37	

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
31	MG	X	3046	-	-	-	X
31	MG	X	3089	-	-	-	X
31	MG	X	3101	-	-	-	X
31	MG	X	3119	-	-	-	X
31	MG	X	3173	-	-	-	X
31	MG	X	3185	-	-	-	X
31	MG	X	3186	-	-	-	X
31	MG	X	3409	-	-	-	X
31	MG	X	3411	-	-	-	X
31	MG	X	3412	-	-	-	X
32	MN	X	3040	-	-	-	X
32	MN	X	3085	-	-	-	X
32	MN	X	3142	-	-	-	X
32	MN	X	3184	-	-	-	X
32	MN	X	3197	-	-	-	X
32	MN	X	3198	-	-	-	X
32	MN	X	3228	-	-	-	X
32	MN	X	3231	-	-	-	X
32	MN	X	3249	-	-	-	X
32	MN	X	3316	-	-	-	X
32	MN	X	3320	-	-	-	X
32	MN	X	3356	-	-	-	X
32	MN	X	3361	-	-	-	X
32	MN	X	3394	-	-	-	X
34	SPD	X	3425	-	-	-	X
34	SPD	X	3434	-	-	X	-
35	EOH	W	102	-	-	-	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
7	E	156	Total	C	N	O	S	0	0	0
			934	571	176	186	1			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

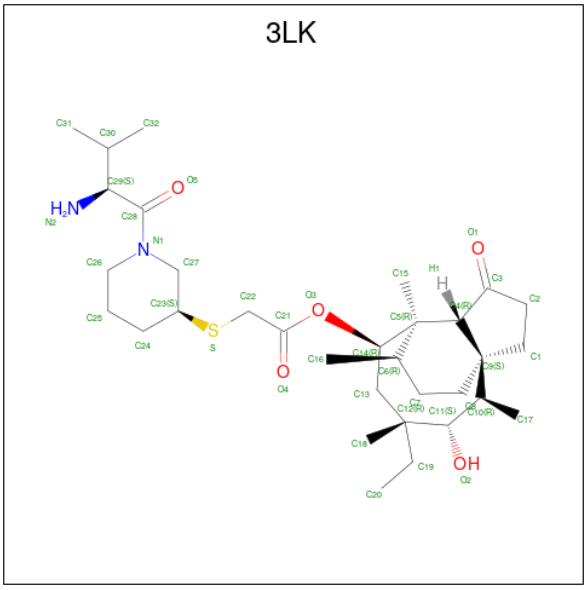
- Molecule 27 is a protein called 50S ribosomal protein L35.

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

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

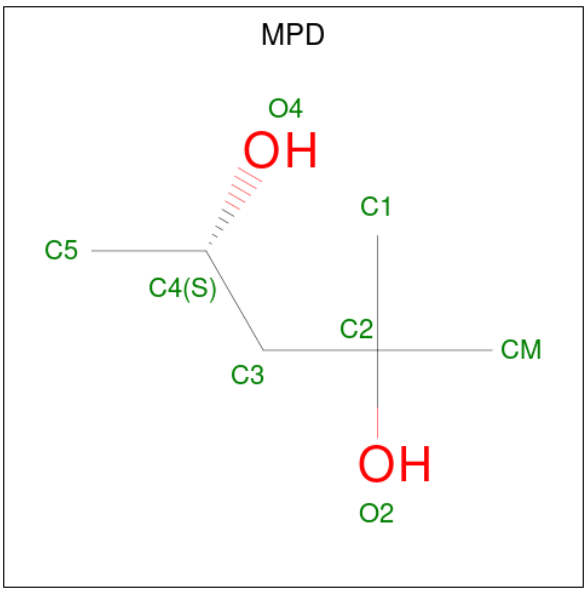
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	4	37	Total	C	N	O	S	0	0	0
			245	149	51	41	4			

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



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

- Molecule 30 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: 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

- Molecule 31 is MAGNESIUM ION (three-letter code: 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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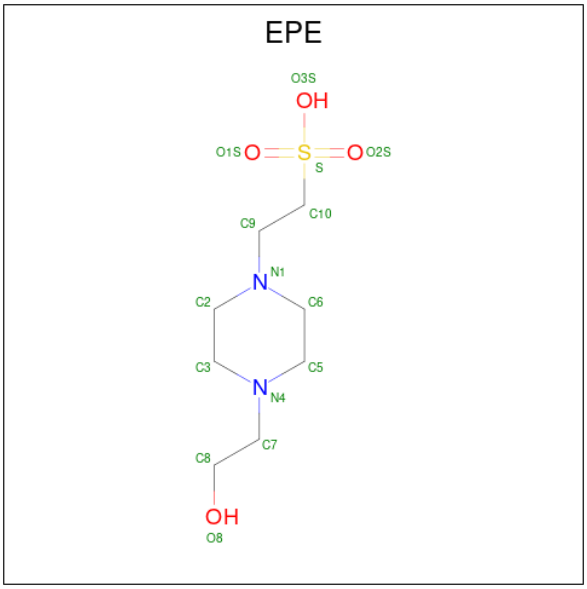
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	E	1	Total Mg 1 1	0	0
31	G	1	Total Mg 1 1	0	0
31	O	1	Total Mg 1 1	0	0

- Molecule 32 is MANGANESE (II) ION (three-letter code: 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 (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



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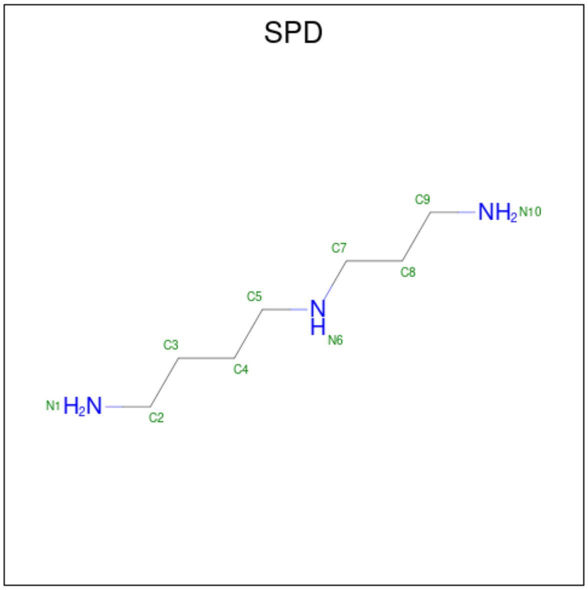
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
33	X	1	Total 15	C 8	N 2	O 4	S 1	0	0
33	X	1	Total 15	C 8	N 2	O 4	S 1	0	0

- Molecule 34 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



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

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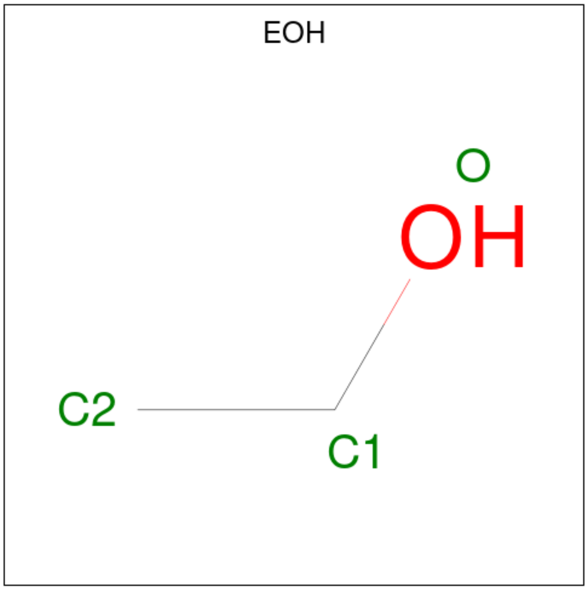
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	X	1	Total 10	C 7	N 3	0	0
34	C	1	Total 10	C 7	N 3	0	0

- Molecule 35 is ETHANOL (three-letter code: EOH) (formula: C_2H_6O).



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

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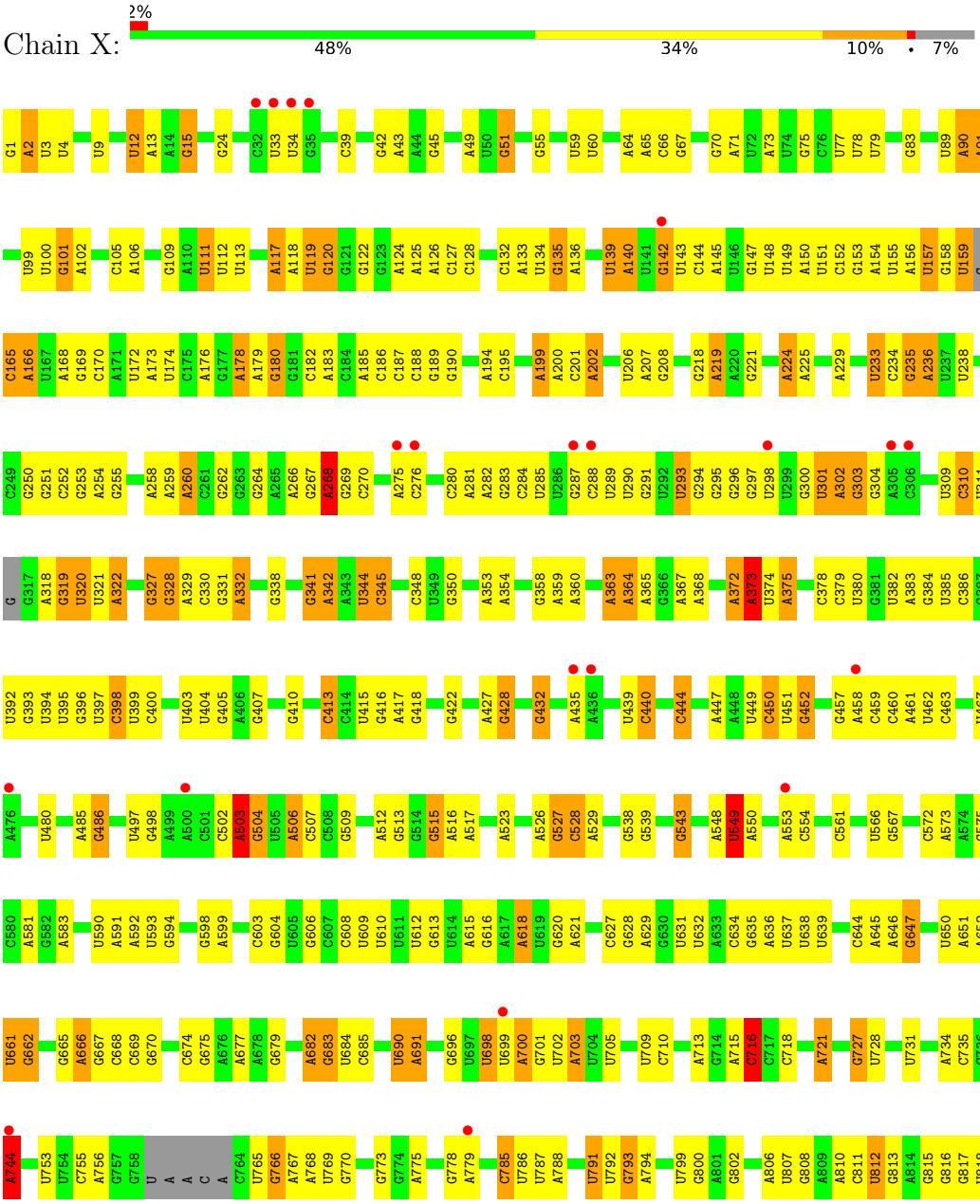
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	Y	1	Total C O 3 2 1	0	0
35	K	1	Total C O 3 2 1	0	0
35	W	1	Total C O 3 2 1	0	0
35	W	1	Total C O 3 2 1	0	0

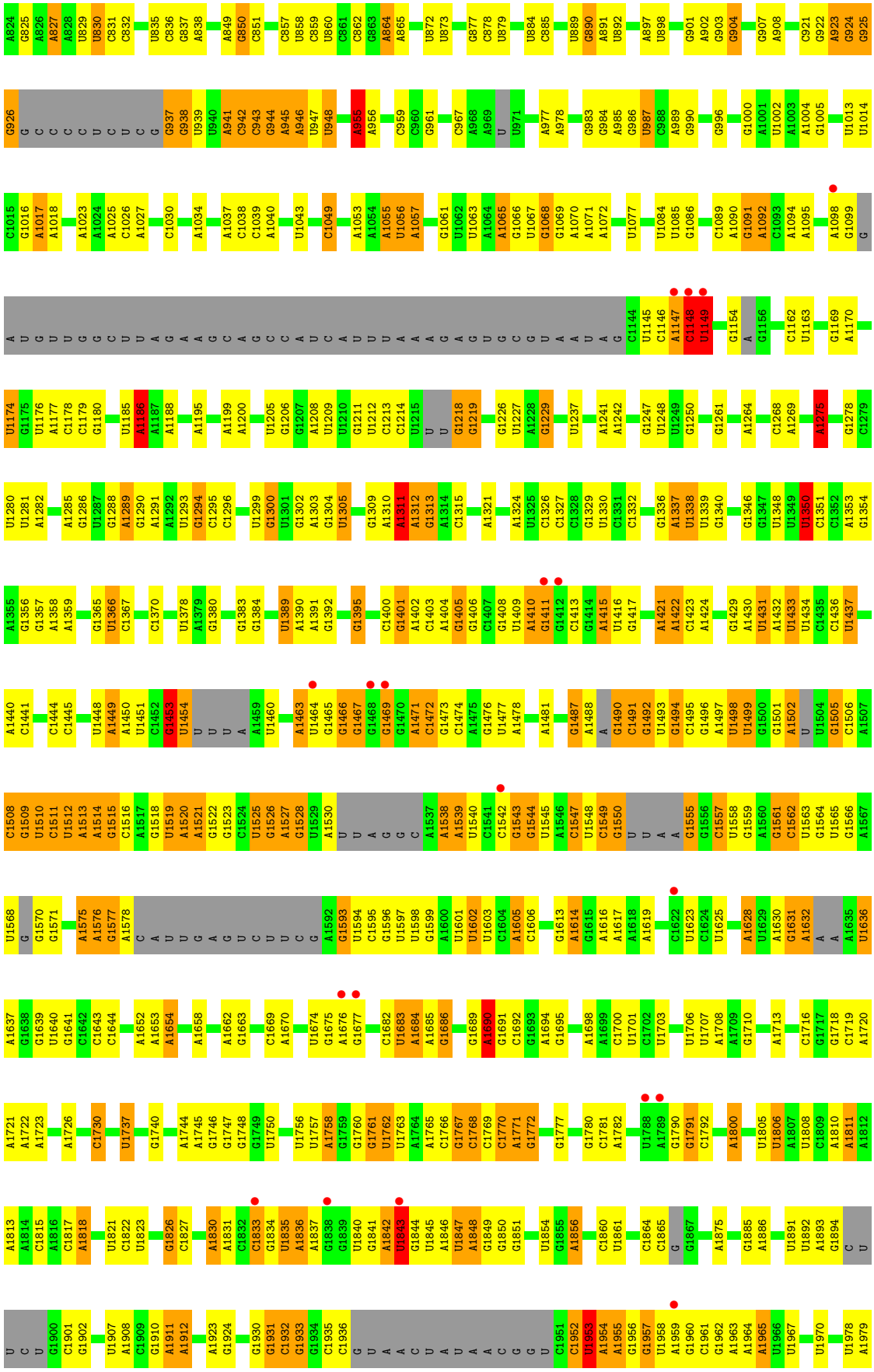
3 Residue-property plots (i)

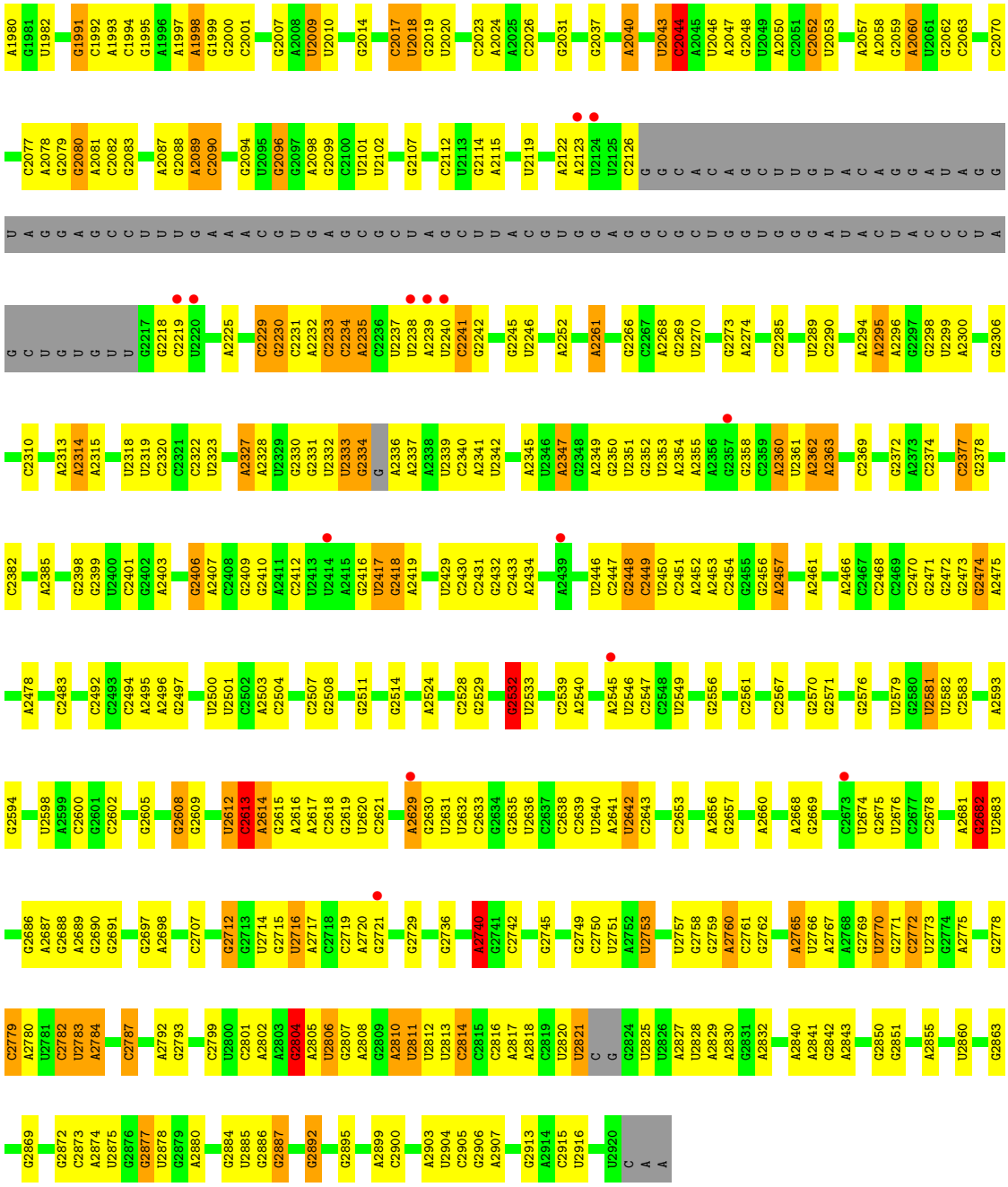
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

Chain X:

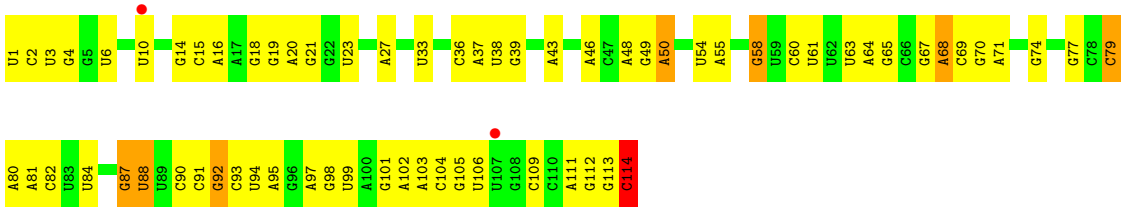






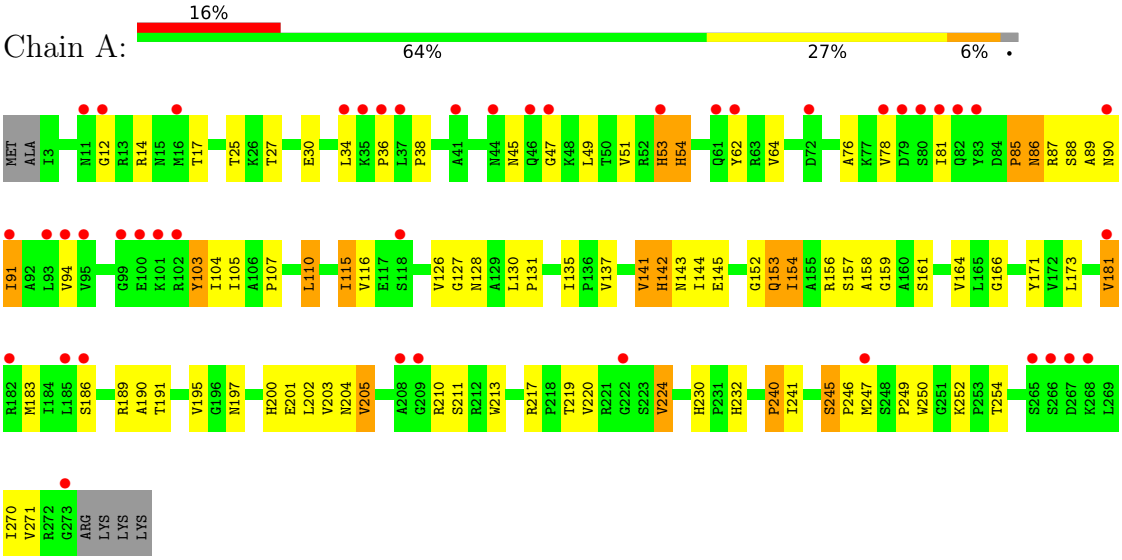
• Molecule 2: 5S rRNA

Chain Y:



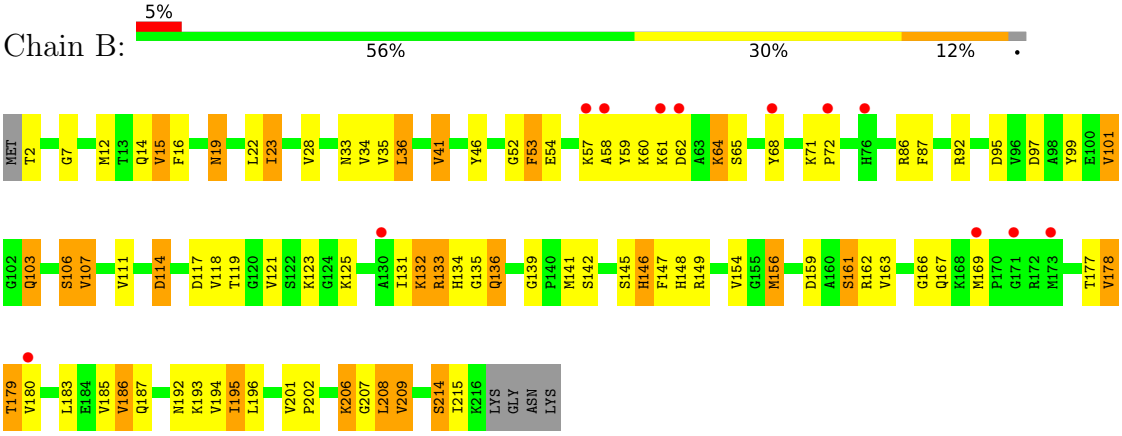
• Molecule 3: 50S ribosomal protein L2

Chain A:



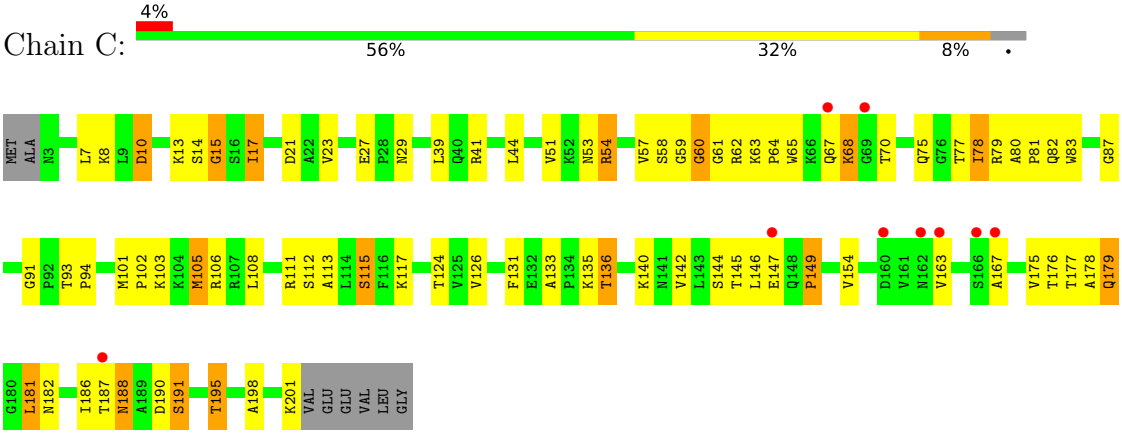
• Molecule 4: 50S ribosomal protein L3

Chain B:



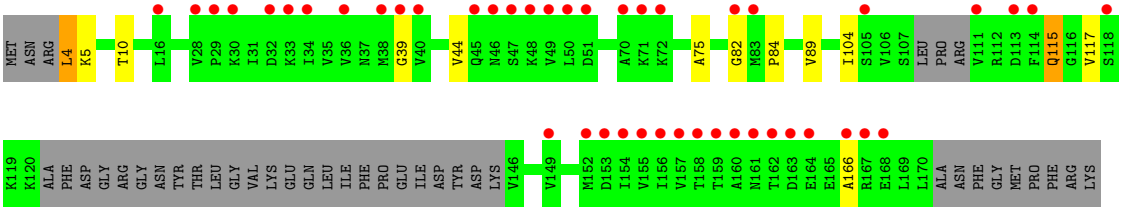
• Molecule 5: 50S ribosomal protein L4

Chain C:



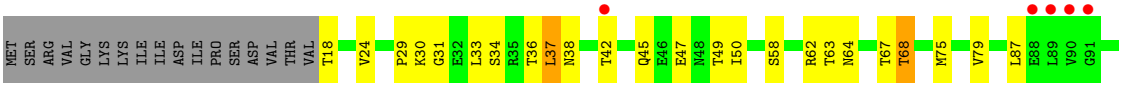
• Molecule 6: 50S ribosomal protein L5

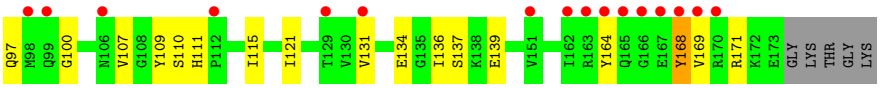
Chain D:



• Molecule 7: 50S ribosomal protein L6

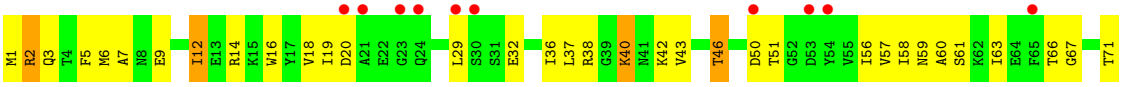
Chain E:

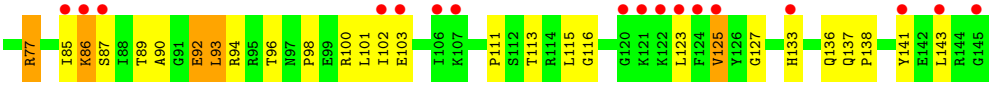




• Molecule 8: 50S ribosomal protein L13

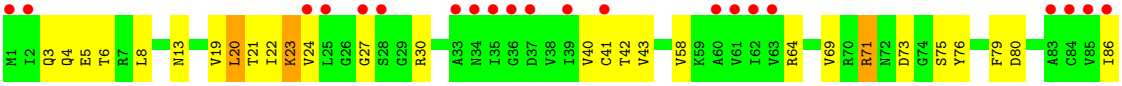
Chain G:

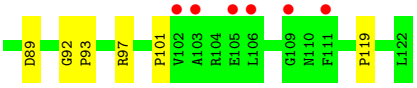




• Molecule 9: 50S ribosomal protein L14

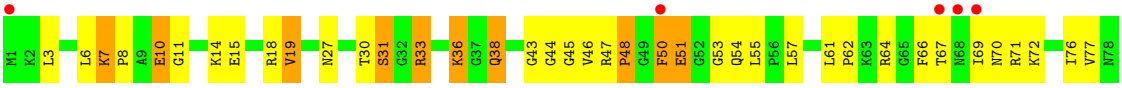
Chain H:

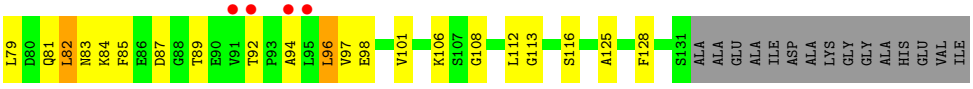




• Molecule 10: 50S ribosomal protein L15

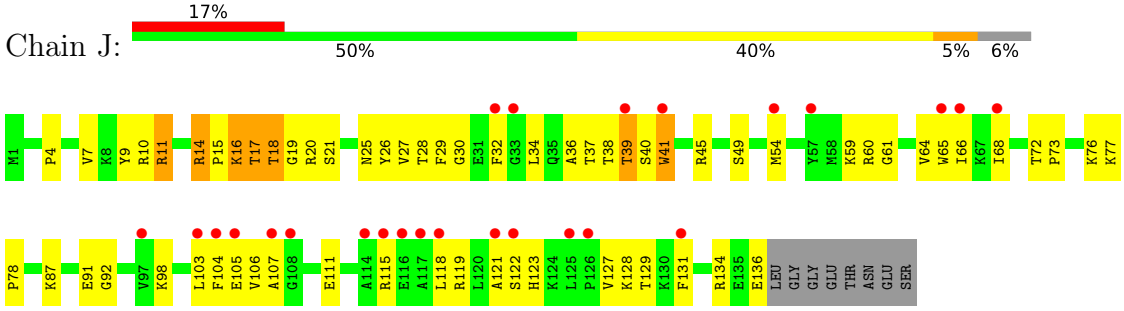
Chain I:





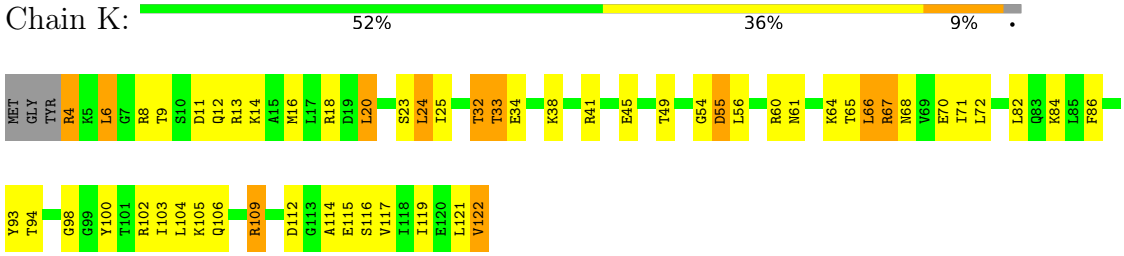
• Molecule 11: 50S ribosomal protein L16

Chain J:



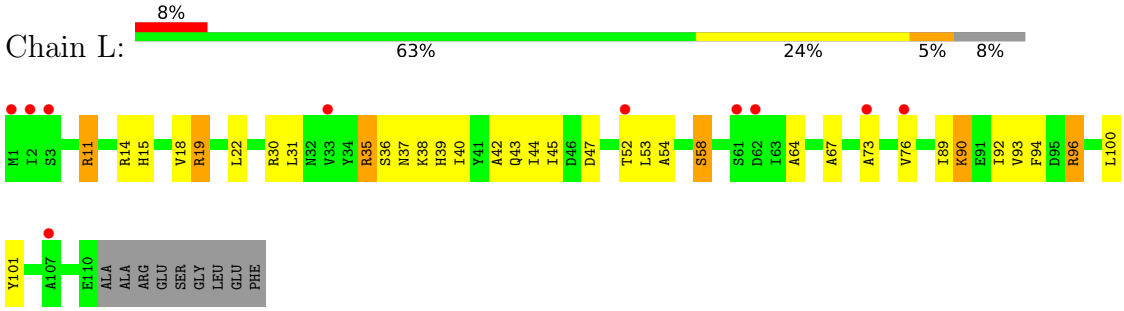
• Molecule 12: 50S ribosomal protein L17

Chain K:



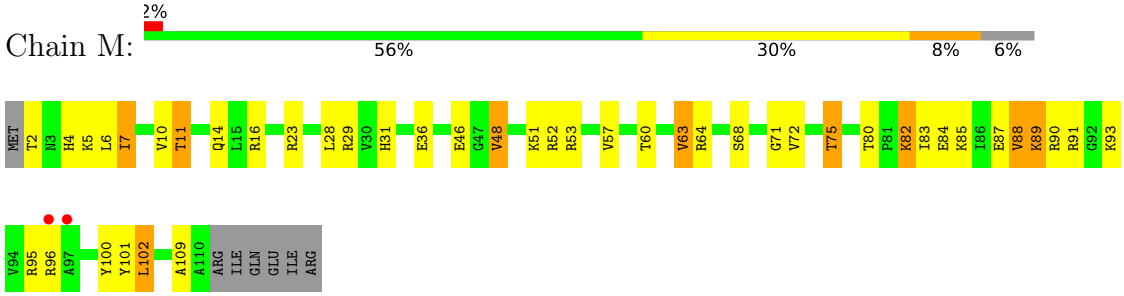
• Molecule 13: 50S ribosomal protein L18

Chain L:



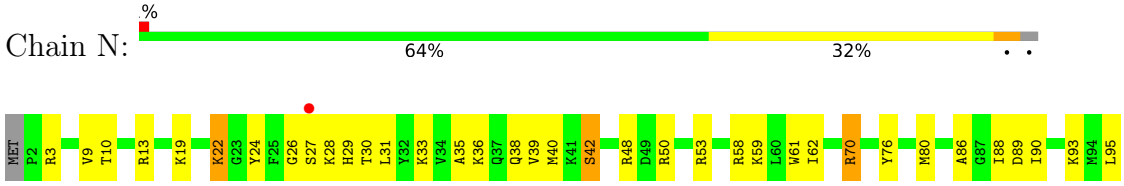
• Molecule 14: 50S ribosomal protein L19

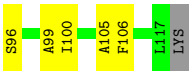
Chain M:



• Molecule 15: 50S ribosomal protein L20

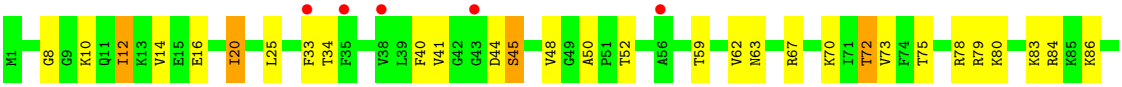
Chain N:

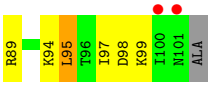




• Molecule 16: 50S ribosomal protein L21

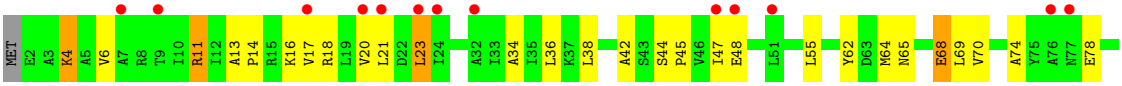
Chain O:

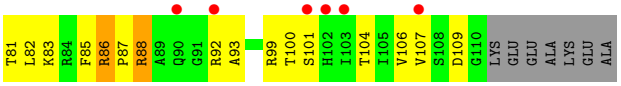




• Molecule 17: 50S ribosomal protein L22

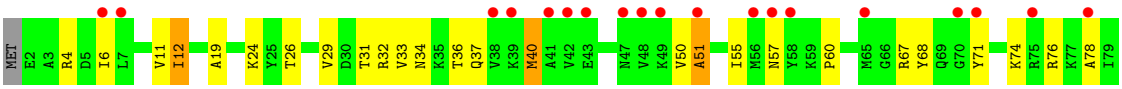
Chain P:

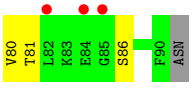




• Molecule 18: 50S ribosomal protein L23

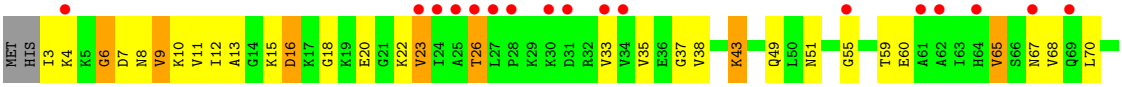
Chain Q:

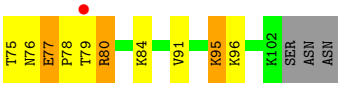




• Molecule 19: 50S ribosomal protein L24

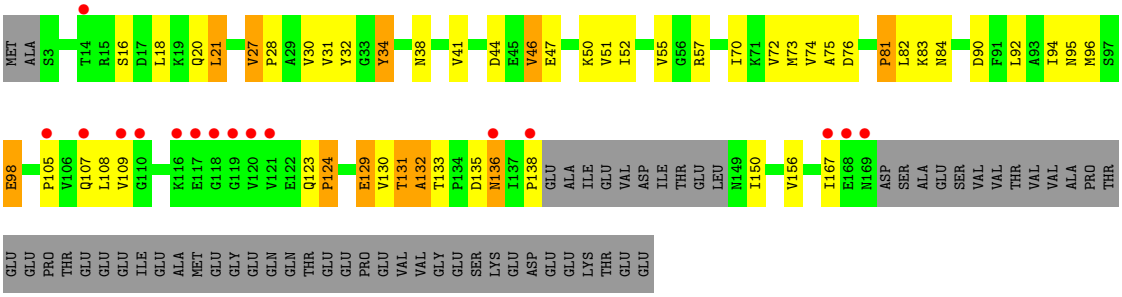
Chain R:



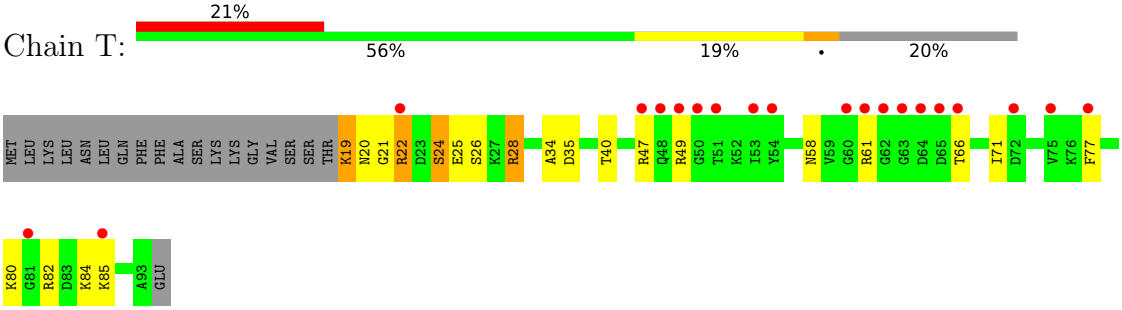


• Molecule 20: 50S ribosomal protein L25

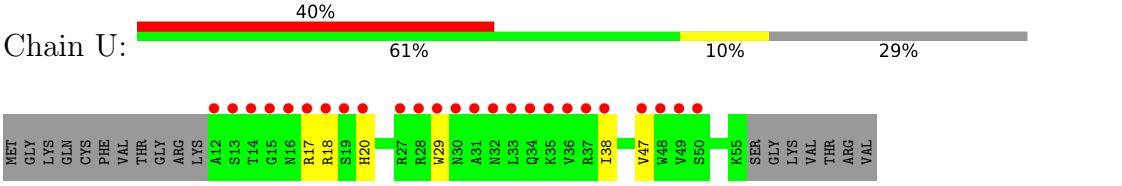
Chain S:



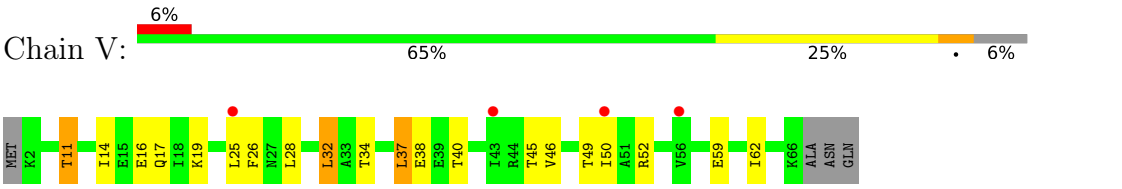
• Molecule 21: 50S ribosomal protein L27



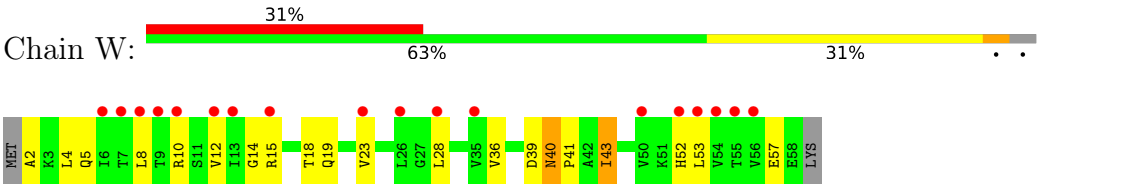
• Molecule 22: 50S ribosomal protein L28



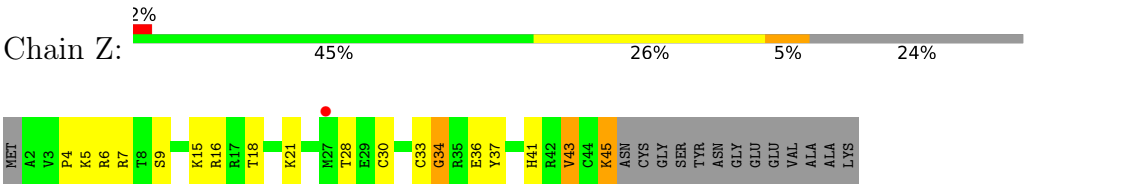
• Molecule 23: 50S ribosomal protein L29



• Molecule 24: 50S ribosomal protein L30

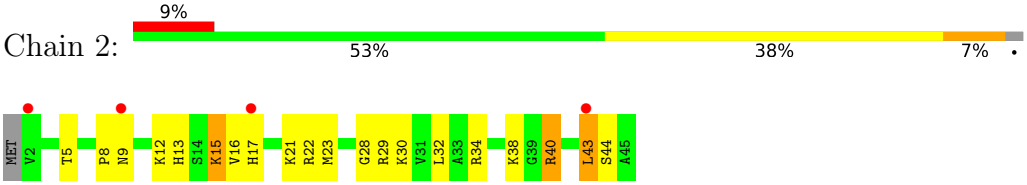


• Molecule 25: 50S ribosomal protein L32



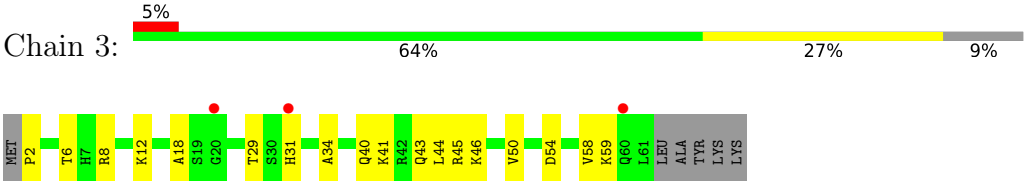
• Molecule 26: 50S ribosomal protein L34

Chain 2:



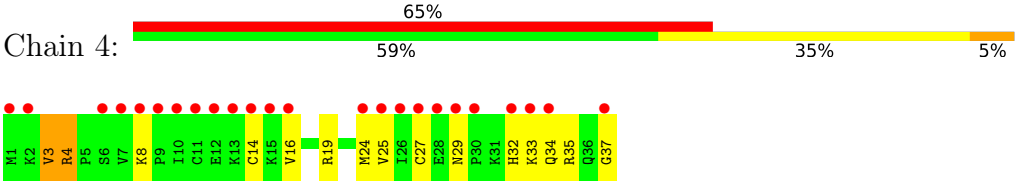
• Molecule 27: 50S ribosomal protein L35

Chain 3:



• Molecule 28: 50S ribosomal protein L36

Chain 4:



4 Data and refinement statistics (i)

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 – 3.41	Depositor EDS
% Data completeness (in resolution range)	91.8 (49.54-3.43) 91.8 (49.54-3.41)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.72 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.204 , 0.242 0.204 , 0.241	Depositor DCC
R_{free} test set	12763 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	98.3	Xtriage
Anisotropy	0.249	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.20 , 62.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	81184	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

Xtriage'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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.57	13/64978 (0.0%)	1.06	182/101293 (0.2%)
2	Y	0.54	0/2717	1.12	16/4232 (0.4%)
3	A	0.32	0/1635	0.62	0/2256
4	B	0.50	0/1570	0.78	0/2116
5	C	0.44	0/1337	0.67	0/1829
6	D	0.26	0/704	0.53	0/973
7	E	0.31	0/943	0.57	0/1301
8	G	0.45	0/1105	0.65	0/1498
9	H	0.42	0/830	0.66	1/1125 (0.1%)
10	I	0.47	0/827	0.84	0/1120
11	J	0.42	0/1037	0.69	0/1404
12	K	0.42	0/889	0.73	1/1192 (0.1%)
13	L	0.33	0/683	0.60	0/935
14	M	0.45	0/834	0.68	0/1125
15	N	0.57	0/944	0.75	0/1252
16	O	0.44	0/748	0.70	0/1007
17	P	0.47	0/831	0.68	0/1122
18	Q	0.35	0/577	0.59	0/791
19	R	0.39	0/611	0.65	0/837
20	S	0.40	0/1030	0.60	0/1412
21	T	0.39	0/545	0.64	0/728
22	U	0.28	0/249	0.56	0/345
23	V	0.37	0/460	0.57	0/621
24	W	0.45	0/415	0.69	0/565
25	Z	0.49	0/347	0.75	0/461
26	2	0.41	0/351	0.66	0/461
27	3	0.56	0/409	0.84	1/547 (0.2%)
28	4	0.36	0/246	0.62	0/330
All	All	0.54	13/87852 (0.0%)	0.99	201/132878 (0.2%)

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

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	577	A	N9-C4	-9.63	1.32	1.37
1	X	1065	A	N9-C4	-7.39	1.33	1.37
1	X	577	A	N3-C4	-7.27	1.30	1.34
1	X	1690	A	N9-C4	6.75	1.42	1.37
1	X	2081	A	N9-C4	-6.54	1.33	1.37

The worst 5 of 201 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	577	A	C2-N3-C4	-12.95	104.13	110.60
1	X	1065	A	C2-N3-C4	-12.08	104.56	110.60
1	X	2048	G	N3-C4-C5	10.50	133.85	128.60
1	X	577	A	N1-C6-N6	10.14	124.68	118.60
2	Y	93	C	N3-C2-O2	-10.03	114.88	121.90

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	788	1
2	Y	2430	0	1229	50	0
3	A	1608	0	1202	51	0
4	B	1547	0	1526	59	0
5	C	1318	0	1167	47	0
6	D	707	0	349	3	0
7	E	934	0	679	13	0
8	G	1083	0	1030	47	0
9	H	824	0	766	17	0
10	I	820	0	678	30	0
11	J	1013	0	993	36	0
12	K	886	0	889	31	0
13	L	678	0	547	27	0
14	M	822	0	837	29	0
15	N	932	0	997	31	0
16	O	738	0	716	19	0
17	P	823	0	866	30	0
18	Q	572	0	456	16	0
19	R	607	0	489	24	0
20	S	1020	0	868	20	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	11	0
25	Z	342	0	345	17	0
26	2	348	0	373	16	0
27	3	405	0	367	8	0
28	4	245	0	215	10	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	C	10	0	19	1	0
34	X	100	0	190	12	0
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	1313	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 1313 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:79:U:HO2'	1:X:389:A:H8	1.03	0.97
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

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%)	1 8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	B	213/220 (97%)	181 (85%)	19 (9%)	13 (6%)	1 13
5	C	197/207 (95%)	168 (85%)	18 (9%)	11 (6%)	2 16
6	D	133/179 (74%)	112 (84%)	13 (10%)	8 (6%)	1 14
7	E	154/178 (86%)	112 (73%)	30 (20%)	12 (8%)	1 9
8	G	143/145 (99%)	125 (87%)	14 (10%)	4 (3%)	5 31
9	H	120/122 (98%)	110 (92%)	7 (6%)	3 (2%)	5 33
10	I	129/146 (88%)	88 (68%)	24 (19%)	17 (13%)	0 3
11	J	134/144 (93%)	117 (87%)	10 (8%)	7 (5%)	2 17
12	K	117/122 (96%)	98 (84%)	12 (10%)	7 (6%)	1 14
13	L	108/119 (91%)	94 (87%)	10 (9%)	4 (4%)	3 25
14	M	107/116 (92%)	90 (84%)	11 (10%)	6 (6%)	2 16
15	N	114/118 (97%)	111 (97%)	2 (2%)	1 (1%)	17 54
16	O	99/102 (97%)	86 (87%)	6 (6%)	7 (7%)	1 10
17	P	107/117 (92%)	102 (95%)	5 (5%)	0	100 100
18	Q	87/91 (96%)	80 (92%)	4 (5%)	3 (3%)	3 27
19	R	98/105 (93%)	75 (76%)	14 (14%)	9 (9%)	1 7
20	S	153/217 (70%)	121 (79%)	19 (12%)	13 (8%)	1 8
21	T	73/94 (78%)	65 (89%)	5 (7%)	3 (4%)	3 23
22	U	42/62 (68%)	31 (74%)	9 (21%)	2 (5%)	2 19
23	V	63/69 (91%)	61 (97%)	1 (2%)	1 (2%)	9 42
24	W	55/59 (93%)	51 (93%)	3 (6%)	1 (2%)	8 39
25	Z	42/58 (72%)	36 (86%)	5 (12%)	1 (2%)	6 34
26	2	42/45 (93%)	39 (93%)	3 (7%)	0	100 100
27	3	58/66 (88%)	44 (76%)	7 (12%)	7 (12%)	0 4
28	4	35/37 (95%)	32 (91%)	2 (6%)	1 (3%)	4 30
All	All	2892/3215 (90%)	2445 (84%)	283 (10%)	164 (6%)	1 15

5 of 164 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	38	PRO
3	A	51	VAL
3	A	156	ARG

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Mol	Chain	Res	Type
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%)	85 (88%)	11 (12%)	5 25
4	B	150/177 (85%)	117 (78%)	33 (22%)	1 4
5	C	104/169 (62%)	81 (78%)	23 (22%)	1 4
6	D	9/158 (6%)	7 (78%)	2 (22%)	1 4
7	E	56/155 (36%)	42 (75%)	14 (25%)	0 3
8	G	104/123 (85%)	86 (83%)	18 (17%)	2 10
9	H	73/100 (73%)	64 (88%)	9 (12%)	4 22
10	I	54/112 (48%)	37 (68%)	17 (32%)	0 2
11	J	95/119 (80%)	78 (82%)	17 (18%)	2 8
12	K	85/102 (83%)	68 (80%)	17 (20%)	1 5
13	L	40/95 (42%)	32 (80%)	8 (20%)	1 5
14	M	81/102 (79%)	65 (80%)	16 (20%)	1 5
15	N	93/98 (95%)	82 (88%)	11 (12%)	5 23
16	O	69/86 (80%)	58 (84%)	11 (16%)	2 13
17	P	84/94 (89%)	72 (86%)	12 (14%)	3 17
18	Q	39/82 (48%)	33 (85%)	6 (15%)	2 14
19	R	42/90 (47%)	30 (71%)	12 (29%)	0 2
20	S	82/190 (43%)	67 (82%)	15 (18%)	1 7
21	T	48/75 (64%)	42 (88%)	6 (12%)	4 21
22	U	7/52 (14%)	6 (86%)	1 (14%)	3 17
23	V	40/62 (64%)	31 (78%)	9 (22%)	1 3
24	W	43/53 (81%)	38 (88%)	5 (12%)	5 24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
25	Z	36/51 (71%)	31 (86%)	5 (14%)	3 18
26	2	34/40 (85%)	28 (82%)	6 (18%)	2 9
27	3	32/57 (56%)	28 (88%)	4 (12%)	4 21
28	4	20/35 (57%)	16 (80%)	4 (20%)	1 5
All	All	1616/2701 (60%)	1324 (82%)	292 (18%)	1 8

5 of 292 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
19	R	65	VAL
27	3	40	GLN
20	S	20	GLN
23	V	19	LYS
8	G	101	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2686/2923 (91%)	622 (23%)	26 (0%)
2	Y	113/114 (99%)	16 (14%)	0
All	All	2799/3037 (92%)	638 (22%)	26 (0%)

5 of 638 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
1	X	1954	A

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Mol	Chain	Res	Type
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 monosaccharides 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	$\#\|Z\| > 2$
34	SPD	X	3431	-	9,9,9	0.11	0	8,8,8	0.09	0
34	SPD	X	3427	-	9,9,9	0.18	0	8,8,8	0.26	0
35	EOH	W	102	-	2,2,2	0.52	0	1,1,1	0.65	0
34	SPD	X	3428	-	9,9,9	0.18	0	8,8,8	0.18	0
34	SPD	C	302	-	9,9,9	0.23	0	8,8,8	0.19	0
30	MPD	X	3010	-	7,7,7	0.33	0	9,10,10	0.12	0
30	MPD	X	3013	-	7,7,7	0.45	0	9,10,10	0.15	0
34	SPD	X	3434	-	9,9,9	0.06	0	8,8,8	0.28	0
35	EOH	X	3439	-	2,2,2	0.50	0	1,1,1	0.81	0
30	MPD	X	3006	-	7,7,7	0.65	0	9,10,10	0.27	0
35	EOH	X	3438	-	2,2,2	0.53	0	1,1,1	0.63	0
35	EOH	X	3437	-	2,2,2	0.50	0	1,1,1	0.72	0
35	EOH	X	3443	-	2,2,2	0.55	0	1,1,1	0.61	0
33	EPE	X	3421	-	15,15,15	1.23	1 (6%)	18,20,20	0.21	0
34	SPD	X	3432	-	9,9,9	0.23	0	8,8,8	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
33	EPE	X	3423	-	15,15,15	1.05	1 (6%)	18,20,20	0.86	1 (5%)
34	SPD	X	3430	-	9,9,9	0.17	0	8,8,8	0.34	0
35	EOH	X	3440	-	2,2,2	0.56	0	1,1,1	0.67	0
35	EOH	X	3441	-	2,2,2	0.51	0	1,1,1	0.73	0
30	MPD	X	3016	-	7,7,7	0.80	0	9,10,10	0.56	0
30	MPD	X	3014	-	7,7,7	0.49	0	9,10,10	0.21	0
33	EPE	X	3424	-	15,15,15	0.91	1 (6%)	18,20,20	0.14	0
30	MPD	X	3012	-	7,7,7	0.37	0	9,10,10	0.22	0
35	EOH	K	201	-	2,2,2	0.53	0	1,1,1	0.59	0
35	EOH	W	101	-	2,2,2	0.50	0	1,1,1	0.63	0
30	MPD	X	3009	-	7,7,7	0.61	0	9,10,10	0.18	0
30	MPD	X	3008	-	7,7,7	0.48	0	9,10,10	0.28	0
30	MPD	X	3011	-	7,7,7	0.66	0	9,10,10	0.25	0
35	EOH	X	3435	-	2,2,2	0.56	0	1,1,1	0.61	0
35	EOH	X	3442	-	2,2,2	0.58	0	1,1,1	0.55	0
34	SPD	X	3429	-	9,9,9	0.20	0	8,8,8	0.32	0
30	MPD	X	3015	-	7,7,7	0.32	0	9,10,10	0.18	0
35	EOH	X	3436	-	2,2,2	0.55	0	1,1,1	0.62	0
30	MPD	X	3003	-	7,7,7	0.40	0	9,10,10	0.22	0
33	EPE	X	3422	-	15,15,15	1.02	1 (6%)	18,20,20	0.59	0
30	MPD	X	3004	-	7,7,7	0.35	0	9,10,10	0.24	0
30	MPD	X	3007	-	7,7,7	0.53	0	9,10,10	0.19	0
34	SPD	X	3433	-	9,9,9	0.14	0	8,8,8	0.17	0
34	SPD	X	3426	-	9,9,9	0.17	0	8,8,8	0.12	0
35	EOH	Y	208	-	2,2,2	0.54	0	1,1,1	0.60	0
30	MPD	X	3005	-	7,7,7	0.46	0	9,10,10	0.27	0
34	SPD	X	3425	-	9,9,9	0.19	0	8,8,8	0.22	0
30	MPD	X	3002	-	7,7,7	0.37	0	9,10,10	0.55	0
29	3LK	X	3001	-	40,43,43	1.19	3 (7%)	56,67,67	1.86	8 (14%)

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
34	SPD	X	3431	-	-	1/7/7/7	-
34	SPD	X	3427	-	-	3/7/7/7	-
34	SPD	X	3428	-	-	4/7/7/7	-
34	SPD	C	302	-	-	0/7/7/7	-
30	MPD	X	3010	-	-	0/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	MPD	X	3013	-	-	1/5/5/5	-
34	SPD	X	3434	-	-	2/7/7/7	-
30	MPD	X	3006	-	-	2/5/5/5	-
33	EPE	X	3421	-	-	4/9/19/19	0/1/1/1
34	SPD	X	3432	-	-	3/7/7/7	-
33	EPE	X	3423	-	-	3/9/19/19	0/1/1/1
34	SPD	X	3430	-	-	3/7/7/7	-
30	MPD	X	3016	-	-	1/5/5/5	-
30	MPD	X	3014	-	-	2/5/5/5	-
33	EPE	X	3424	-	-	0/9/19/19	0/1/1/1
30	MPD	X	3012	-	-	2/5/5/5	-
30	MPD	X	3009	-	-	0/5/5/5	-
30	MPD	X	3008	-	-	2/5/5/5	-
30	MPD	X	3011	-	-	3/5/5/5	-
34	SPD	X	3429	-	-	3/7/7/7	-
30	MPD	X	3015	-	-	4/5/5/5	-
30	MPD	X	3003	-	-	2/5/5/5	-
33	EPE	X	3422	-	-	1/9/19/19	0/1/1/1
30	MPD	X	3004	-	-	4/5/5/5	-
30	MPD	X	3007	-	-	1/5/5/5	-
34	SPD	X	3433	-	-	2/7/7/7	-
34	SPD	X	3426	-	-	3/7/7/7	-
30	MPD	X	3005	-	-	2/5/5/5	-
34	SPD	X	3425	-	-	2/7/7/7	-
30	MPD	X	3002	-	-	2/5/5/5	-
29	3LK	X	3001	-	-	3/22/95/95	0/4/4/4

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	X	3001	3LK	C20-C19	-5.69	1.27	1.51
33	X	3421	EPE	C10-S	-4.75	1.70	1.77
33	X	3423	EPE	C10-S	-3.98	1.71	1.77
33	X	3422	EPE	C10-S	-3.79	1.72	1.77
33	X	3424	EPE	C10-S	-3.52	1.72	1.77

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	X	3001	3LK	C20-C19-C12	6.43	126.10	116.21
29	X	3001	3LK	C15-C5-C14	-6.30	102.74	108.95
29	X	3001	3LK	C13-C14-C5	-5.43	110.73	116.31
29	X	3001	3LK	O3-C14-C5	4.46	112.98	106.18
29	X	3001	3LK	C23-C27-N1	-3.44	105.03	109.58

There are no chirality outliers.

5 of 65 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	3006	MPD	C2-C3-C4-C5

There are no ring outliers.

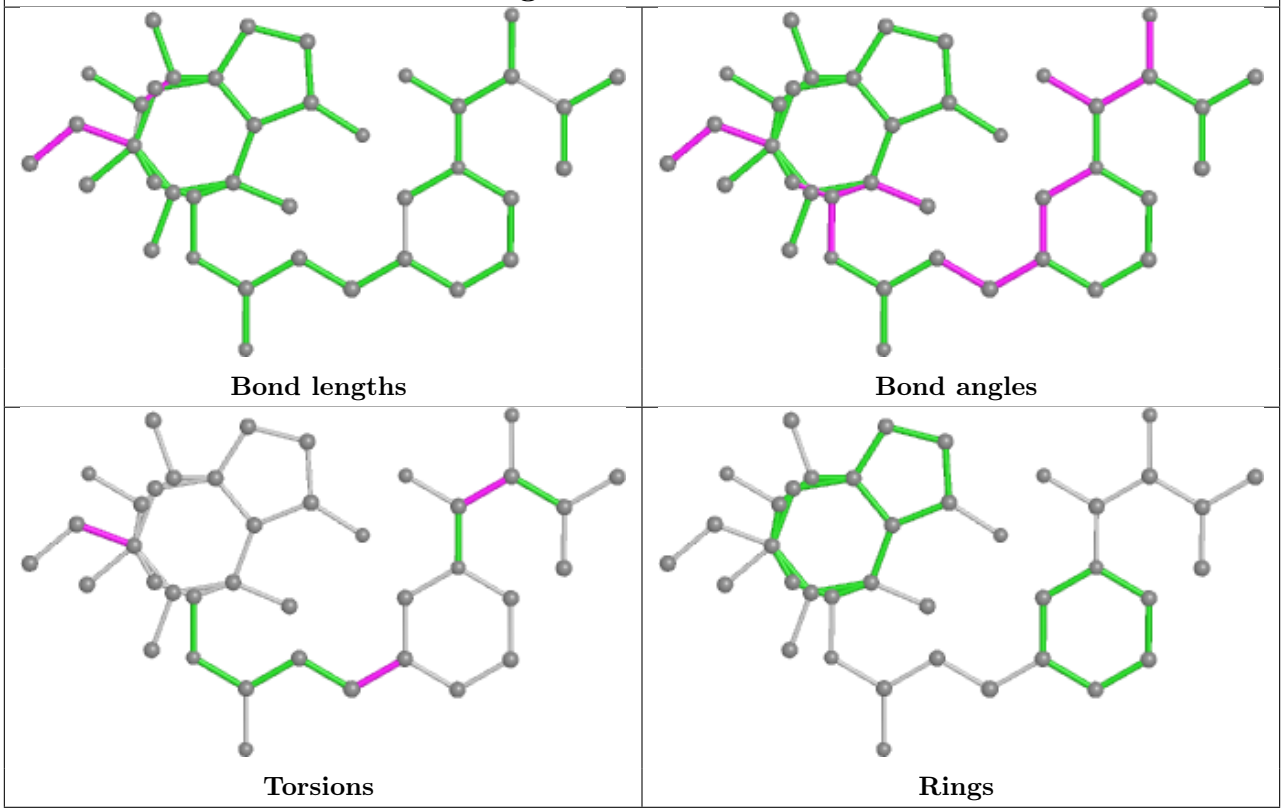
19 monomers are involved in 45 short contacts:

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

Ligand 3LK X 3001



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

6.1 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, 95^{th} 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%)	-0.26	54 (1%) 65 63	26, 70, 166, 275	0
2	Y	114/114 (100%)	-0.34	2 (1%) 68 66	51, 84, 141, 183	0
3	A	271/277 (97%)	0.58	44 (16%) 1 2	54, 100, 155, 195	0
4	B	215/220 (97%)	-0.08	12 (5%) 24 25	34, 49, 101, 134	0
5	C	199/207 (96%)	-0.00	9 (4%) 33 32	37, 60, 111, 160	0
6	D	139/179 (77%)	1.16	45 (32%) 0 0	92, 142, 196, 234	0
7	E	156/178 (87%)	0.07	21 (13%) 3 5	58, 109, 176, 210	0
8	G	145/145 (100%)	0.81	27 (18%) 1 2	37, 49, 76, 133	0
9	H	122/122 (100%)	0.76	27 (22%) 0 1	58, 69, 108, 134	0
10	I	131/146 (89%)	0.02	9 (6%) 16 19	19, 73, 143, 206	0
11	J	136/144 (94%)	0.69	25 (18%) 1 2	41, 65, 127, 172	0
12	K	119/122 (97%)	-0.33	0 100 100	34, 57, 127, 151	0
13	L	110/119 (92%)	0.16	10 (9%) 9 11	56, 87, 131, 174	0
14	M	109/116 (93%)	-0.23	2 (1%) 68 66	47, 64, 135, 177	0
15	N	116/118 (98%)	-0.27	1 (0%) 84 81	24, 39, 87, 129	0
16	O	101/102 (99%)	0.26	7 (6%) 16 19	23, 56, 101, 154	0
17	P	109/117 (93%)	0.71	19 (17%) 1 2	37, 49, 97, 134	0
18	Q	89/91 (97%)	0.81	22 (24%) 0 0	37, 88, 133, 162	0
19	R	100/105 (95%)	0.47	18 (18%) 1 2	35, 90, 171, 210	0
20	S	157/217 (72%)	0.22	16 (10%) 6 9	46, 78, 157, 244	0
21	T	75/94 (79%)	1.05	20 (26%) 0 0	33, 58, 109, 130	0
22	U	44/62 (70%)	2.66	25 (56%) 0 0	78, 120, 166, 218	0
23	V	65/69 (94%)	0.38	4 (6%) 20 22	79, 108, 170, 237	0
24	W	57/59 (96%)	1.29	18 (31%) 0 0	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%)	-0.19	1 (2%) 60 58	28, 51, 130, 153	0
26	2	44/45 (97%)	0.76	4 (9%) 9 11	54, 63, 85, 112	0
27	3	60/66 (90%)	0.26	3 (5%) 28 29	31, 53, 78, 94	0
28	4	37/37 (100%)	2.88	24 (64%) 0 0	56, 78, 106, 118	0
All	All	5771/6252 (92%)	0.08	469 (8%) 12 15	19, 71, 158, 275	0

The worst 5 of 469 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	S	109	VAL	8.4
1	X	2629	A	7.6
22	U	13	SER	7.4
28	4	29	ASN	6.9
28	4	11	CYS	6.5

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 monosaccharides 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
31	MG	X	3101	1/1	0.12	1.10	80,80,80,80	0
31	MG	X	3119	1/1	0.43	0.53	87,87,87,87	0
32	MN	X	3228	1/1	0.52	0.93	190,190,190,190	0
31	MG	X	3173	1/1	0.55	1.26	34,34,34,34	1
31	MG	X	3185	1/1	0.57	0.41	74,74,74,74	0
31	MG	X	3046	1/1	0.59	0.53	67,67,67,67	0
32	MN	X	3040	1/1	0.60	0.70	157,157,157,157	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	MN	X	3361	1/1	0.61	0.42	148,148,148,148	0
32	MN	X	3261	1/1	0.62	0.16	139,139,139,139	0
31	MG	X	3412	1/1	0.62	0.79	73,73,73,73	0
32	MN	X	3231	1/1	0.67	1.12	166,166,166,166	0
31	MG	X	3123	1/1	0.67	0.38	77,77,77,77	0
32	MN	X	3283	1/1	0.67	0.20	121,121,121,121	0
31	MG	X	3089	1/1	0.67	2.39	91,91,91,91	0
32	MN	X	3198	1/1	0.69	0.58	154,154,154,154	0
31	MG	X	3186	1/1	0.69	0.68	15,15,15,15	1
32	MN	X	3157	1/1	0.70	0.16	103,103,103,103	0
31	MG	X	3411	1/1	0.70	1.09	78,78,78,78	0
32	MN	X	3356	1/1	0.70	0.68	95,95,95,95	0
32	MN	X	3249	1/1	0.70	0.50	149,149,149,149	0
32	MN	X	3143	1/1	0.71	0.32	157,157,157,157	0
32	MN	X	3184	1/1	0.71	0.61	139,139,139,139	0
34	SPD	X	3425	10/10	0.73	0.50	101,101,101,101	0
32	MN	X	3316	1/1	0.74	1.29	131,131,131,131	0
31	MG	X	3111	1/1	0.74	0.30	25,25,25,25	0
32	MN	X	3021	1/1	0.74	0.39	118,118,118,118	0
32	MN	R	201	1/1	0.74	0.24	118,118,118,118	0
32	MN	X	3311	1/1	0.74	0.29	140,140,140,140	0
32	MN	X	3394	1/1	0.75	0.68	105,105,105,105	0
31	MG	X	3102	1/1	0.75	0.24	33,33,33,33	0
33	EPE	X	3424	15/15	0.75	0.38	137,137,137,137	0
32	MN	X	3152	1/1	0.75	0.33	136,136,136,136	0
32	MN	X	3404	1/1	0.76	0.20	116,116,116,116	0
32	MN	X	3159	1/1	0.76	0.16	137,137,137,137	0
35	EOH	W	102	3/3	0.76	0.48	66,66,66,66	0
31	MG	X	3168	1/1	0.77	0.38	57,57,57,57	0
31	MG	X	3070	1/1	0.77	0.09	91,91,91,91	0
32	MN	X	3142	1/1	0.77	0.60	166,166,166,166	0
31	MG	O	201	1/1	0.77	0.34	30,30,30,30	0
32	MN	X	3066	1/1	0.78	0.36	146,146,146,146	0
32	MN	X	3253	1/1	0.78	0.27	134,134,134,134	0
31	MG	X	3171	1/1	0.78	0.30	75,75,75,75	0
32	MN	X	3320	1/1	0.78	0.45	91,91,91,91	0
30	MPD	X	3011	8/8	0.79	0.33	106,106,106,106	0
31	MG	X	3052	1/1	0.79	0.32	26,26,26,26	0
31	MG	X	3409	1/1	0.79	0.49	35,35,35,35	1
32	MN	X	3085	1/1	0.79	0.80	185,185,185,185	0
32	MN	X	3197	1/1	0.80	0.73	111,111,111,111	0
32	MN	X	3383	1/1	0.80	0.19	156,156,156,156	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	MPD	X	3014	8/8	0.80	0.30	105,105,105,105	0
34	SPD	X	3433	10/10	0.80	0.31	97,97,97,97	0
35	EOH	X	3437	3/3	0.80	0.68	108,108,108,108	0
32	MN	X	3260	1/1	0.80	0.78	154,154,154,154	0
32	MN	X	3218	1/1	0.81	0.40	170,170,170,170	0
32	MN	X	3354	1/1	0.81	0.29	114,114,114,114	0
33	EPE	X	3422	15/15	0.81	0.50	155,155,155,155	0
31	MG	X	3121	1/1	0.81	0.70	81,81,81,81	0
31	MG	X	3108	1/1	0.81	0.28	74,74,74,74	0
34	SPD	X	3428	10/10	0.81	0.43	55,55,55,55	0
31	MG	X	3126	1/1	0.81	0.39	51,51,51,51	0
35	EOH	X	3436	3/3	0.81	0.80	69,69,69,69	0
32	MN	X	3385	1/1	0.81	0.21	108,108,108,108	0
32	MN	X	3216	1/1	0.81	0.60	128,128,128,128	0
31	MG	X	3112	1/1	0.82	0.20	23,23,23,23	1
32	MN	X	3230	1/1	0.82	0.32	118,118,118,118	0
32	MN	X	3291	1/1	0.82	0.24	90,90,90,90	0
32	MN	X	3399	1/1	0.82	0.54	130,130,130,130	0
31	MG	X	3107	1/1	0.82	0.35	58,58,58,58	0
32	MN	X	3445	1/1	0.82	0.38	108,108,108,108	0
32	MN	A	301	1/1	0.82	0.31	119,119,119,119	0
32	MN	X	3315	1/1	0.82	0.47	143,143,143,143	0
32	MN	Y	205	1/1	0.83	0.14	103,103,103,103	0
32	MN	X	3033	1/1	0.83	0.32	136,136,136,136	0
31	MG	X	3060	1/1	0.83	0.56	42,42,42,42	0
30	MPD	X	3013	8/8	0.83	0.34	95,95,95,95	0
33	EPE	X	3423	15/15	0.83	0.31	145,145,145,145	0
32	MN	X	3362	1/1	0.83	0.28	99,99,99,99	0
31	MG	X	3028	1/1	0.83	1.47	66,66,66,66	0
32	MN	X	3304	1/1	0.83	0.18	81,81,81,81	0
31	MG	X	3092	1/1	0.83	0.87	66,66,66,66	0
32	MN	X	3233	1/1	0.83	0.23	97,97,97,97	0
31	MG	X	3093	1/1	0.83	0.61	77,77,77,77	0
35	EOH	X	3441	3/3	0.83	0.29	82,82,82,82	0
32	MN	X	3199	1/1	0.83	0.30	130,130,130,130	0
31	MG	X	3103	1/1	0.84	0.33	78,78,78,78	0
31	MG	Y	204	1/1	0.84	0.19	57,57,57,57	0
30	MPD	X	3008	8/8	0.84	0.22	98,98,98,98	0
31	MG	X	3176	1/1	0.84	0.42	39,39,39,39	0
31	MG	X	3095	1/1	0.84	0.62	46,46,46,46	0
31	MG	X	3125	1/1	0.84	0.42	46,46,46,46	0
31	MG	X	3026	1/1	0.84	0.73	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
33	EPE	X	3421	15/15	0.84	0.42	117,117,117,117	4
35	EOH	W	101	3/3	0.84	0.54	73,73,73,73	0
31	MG	X	3069	1/1	0.84	0.30	12,12,12,12	1
31	MG	A	302	1/1	0.85	0.60	38,38,38,38	0
31	MG	X	3188	1/1	0.85	0.28	41,41,41,41	0
32	MN	X	3145	1/1	0.85	0.83	136,136,136,136	0
30	MPD	X	3003	8/8	0.85	0.50	82,82,82,82	0
31	MG	X	3167	1/1	0.85	0.46	108,108,108,108	0
32	MN	X	3036	1/1	0.85	0.31	177,177,177,177	0
32	MN	X	3244	1/1	0.85	0.31	138,138,138,138	0
32	MN	X	3160	1/1	0.85	0.33	126,126,126,126	0
32	MN	X	3367	1/1	0.85	0.69	128,128,128,128	0
34	SPD	X	3430	10/10	0.85	0.43	65,65,65,65	0
32	MN	X	3179	1/1	0.85	0.13	140,140,140,140	0
30	MPD	X	3012	8/8	0.85	0.29	87,87,87,87	0
31	MG	Y	203	1/1	0.85	0.71	103,103,103,103	0
32	MN	X	3077	1/1	0.85	0.14	111,111,111,111	0
31	MG	X	3054	1/1	0.85	0.26	64,64,64,64	0
32	MN	X	3210	1/1	0.85	0.41	140,140,140,140	0
32	MN	X	3147	1/1	0.86	0.26	127,127,127,127	0
34	SPD	X	3429	10/10	0.86	0.31	61,61,61,61	0
32	MN	X	3258	1/1	0.86	0.54	132,132,132,132	0
31	MG	X	3226	1/1	0.86	0.84	57,57,57,57	0
32	MN	X	3202	1/1	0.86	0.44	151,151,151,151	0
32	MN	X	3346	1/1	0.86	0.27	83,83,83,83	0
31	MG	X	3182	1/1	0.86	0.33	66,66,66,66	0
32	MN	X	3190	1/1	0.86	0.38	151,151,151,151	0
31	MG	X	3129	1/1	0.86	1.23	54,54,54,54	0
32	MN	X	3255	1/1	0.87	1.22	217,217,217,217	0
32	MN	X	3209	1/1	0.87	0.50	157,157,157,157	0
32	MN	X	3139	1/1	0.87	0.07	132,132,132,132	0
32	MN	X	3025	1/1	0.87	0.47	130,130,130,130	0
32	MN	X	3374	1/1	0.87	0.29	69,69,69,69	0
34	SPD	X	3426	10/10	0.87	0.43	71,71,71,71	0
32	MN	X	3180	1/1	0.87	0.44	139,139,139,139	0
32	MN	X	3223	1/1	0.87	0.44	131,131,131,131	0
30	MPD	X	3010	8/8	0.87	0.31	129,129,129,129	0
31	MG	X	3055	1/1	0.87	0.28	50,50,50,50	0
31	MG	X	3115	1/1	0.87	0.17	58,58,58,58	0
31	MG	X	3124	1/1	0.87	0.32	50,50,50,50	0
35	EOH	X	3438	3/3	0.87	0.32	77,77,77,77	0
32	MN	X	3020	1/1	0.87	0.88	120,120,120,120	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
35	EOH	Y	208	3/3	0.87	0.73	89,89,89,89	0
31	MG	X	3118	1/1	0.87	0.23	59,59,59,59	0
32	MN	X	3205	1/1	0.87	0.25	101,101,101,101	0
32	MN	X	3194	1/1	0.88	1.18	177,177,177,177	0
31	MG	X	3416	1/1	0.88	0.48	16,16,16,16	0
32	MN	X	3132	1/1	0.88	0.23	112,112,112,112	0
32	MN	X	3134	1/1	0.88	0.34	122,122,122,122	0
31	MG	X	3058	1/1	0.88	0.50	95,95,95,95	0
32	MN	X	3397	1/1	0.88	0.16	106,106,106,106	0
31	MG	X	3109	1/1	0.88	0.20	46,46,46,46	0
32	MN	X	3403	1/1	0.88	0.27	98,98,98,98	0
34	SPD	C	302	10/10	0.88	0.26	0,0,0,0	10
31	MG	X	3414	1/1	0.88	0.57	64,64,64,64	0
32	MN	X	3333	1/1	0.88	0.39	117,117,117,117	0
32	MN	X	3183	1/1	0.88	0.35	145,145,145,145	0
32	MN	X	3032	1/1	0.88	0.18	170,170,170,170	0
32	MN	X	3079	1/1	0.88	0.66	145,145,145,145	0
32	MN	X	3219	1/1	0.88	0.14	119,119,119,119	0
32	MN	X	3222	1/1	0.88	0.81	150,150,150,150	0
32	MN	X	3378	1/1	0.89	0.89	141,141,141,141	0
32	MN	X	3191	1/1	0.89	0.21	75,75,75,75	0
32	MN	X	3349	1/1	0.89	0.24	99,99,99,99	0
30	MPD	X	3006	8/8	0.89	0.33	110,110,110,110	0
32	MN	X	3181	1/1	0.89	0.12	91,91,91,91	0
32	MN	X	3360	1/1	0.89	0.38	122,122,122,122	0
35	EOH	X	3439	3/3	0.89	0.25	64,64,64,64	0
32	MN	X	3215	1/1	0.89	0.15	101,101,101,101	0
35	EOH	X	3442	3/3	0.89	1.00	68,68,68,68	0
32	MN	X	3019	1/1	0.89	0.52	148,148,148,148	0
32	MN	X	3162	1/1	0.89	0.33	130,130,130,130	0
32	MN	X	3076	1/1	0.89	0.21	144,144,144,144	0
32	MN	X	3254	1/1	0.90	0.29	106,106,106,106	0
32	MN	X	3357	1/1	0.90	0.81	134,134,134,134	0
31	MG	X	3413	1/1	0.90	0.19	52,52,52,52	0
31	MG	X	3130	1/1	0.90	0.23	65,65,65,65	0
32	MN	X	3086	1/1	0.90	0.10	122,122,122,122	0
32	MN	X	3192	1/1	0.90	0.34	125,125,125,125	0
34	SPD	X	3427	10/10	0.90	0.46	72,72,72,72	0
32	MN	X	3273	1/1	0.90	0.21	35,35,35,35	0
32	MN	X	3220	1/1	0.90	0.35	133,133,133,133	0
32	MN	X	3090	1/1	0.90	0.19	114,114,114,114	0
32	MN	X	3301	1/1	0.90	0.22	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
34	SPD	X	3434	10/10	0.90	0.25	91,91,91,91	0
32	MN	X	3195	1/1	0.90	0.43	129,129,129,129	0
32	MN	X	3395	1/1	0.90	0.44	117,117,117,117	0
32	MN	X	3224	1/1	0.90	0.13	104,104,104,104	0
31	MG	X	3117	1/1	0.90	0.47	34,34,34,34	0
32	MN	X	3133	1/1	0.90	0.46	139,139,139,139	0
32	MN	X	3041	1/1	0.90	0.24	185,185,185,185	0
32	MN	X	3023	1/1	0.90	0.69	193,193,193,193	0
32	MN	X	3141	1/1	0.90	0.28	127,127,127,127	0
31	MG	B	302	1/1	0.90	0.25	34,34,34,34	0
31	MG	X	3418	1/1	0.90	0.49	51,51,51,51	0
32	MN	X	3088	1/1	0.91	0.41	149,149,149,149	0
32	MN	X	3313	1/1	0.91	0.34	88,88,88,88	0
32	MN	X	3381	1/1	0.91	0.24	102,102,102,102	0
32	MN	X	3382	1/1	0.91	0.28	140,140,140,140	0
31	MG	X	3048	1/1	0.91	0.15	49,49,49,49	0
32	MN	X	3098	1/1	0.91	0.19	143,143,143,143	0
32	MN	X	3389	1/1	0.91	0.09	105,105,105,105	0
31	MG	G	201	1/1	0.91	0.20	49,49,49,49	0
32	MN	X	3203	1/1	0.91	0.21	96,96,96,96	0
31	MG	X	3071	1/1	0.91	0.45	100,100,100,100	0
32	MN	X	3269	1/1	0.91	0.23	71,71,71,71	0
32	MN	X	3352	1/1	0.91	0.18	142,142,142,142	0
31	MG	X	3050	1/1	0.91	0.64	83,83,83,83	0
32	MN	X	3034	1/1	0.91	0.45	182,182,182,182	0
32	MN	Y	202	1/1	0.91	0.14	124,124,124,124	0
30	MPD	X	3005	8/8	0.91	0.22	99,99,99,99	0
32	MN	X	3300	1/1	0.91	0.32	107,107,107,107	0
30	MPD	X	3009	8/8	0.91	0.20	91,91,91,91	0
32	MN	X	3196	1/1	0.91	0.25	88,88,88,88	0
32	MN	X	3308	1/1	0.91	0.54	103,103,103,103	0
31	MG	X	3105	1/1	0.92	0.16	56,56,56,56	0
31	MG	X	3177	1/1	0.92	0.72	64,64,64,64	0
32	MN	X	3018	1/1	0.92	0.55	116,116,116,116	0
30	MPD	X	3002	8/8	0.92	0.20	56,56,56,56	0
32	MN	X	3212	1/1	0.92	0.32	106,106,106,106	0
32	MN	X	3075	1/1	0.92	0.48	136,136,136,136	0
32	MN	X	3327	1/1	0.92	0.24	99,99,99,99	0
30	MPD	X	3007	8/8	0.92	0.43	87,87,87,87	0
31	MG	X	3051	1/1	0.92	0.41	64,64,64,64	0
31	MG	X	3110	1/1	0.92	0.18	51,51,51,51	0
32	MN	X	3264	1/1	0.92	0.49	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	MN	X	3082	1/1	0.92	0.29	48,48,48,48	0
31	MG	X	3122	1/1	0.92	0.23	92,92,92,92	0
31	MG	Y	207	1/1	0.92	0.89	20,20,20,20	1
31	MG	X	3056	1/1	0.92	0.34	68,68,68,68	0
31	MG	X	3104	1/1	0.92	0.20	42,42,42,42	0
32	MN	X	3161	1/1	0.92	0.26	70,70,70,70	0
35	EOH	X	3443	3/3	0.92	0.48	59,59,59,59	0
32	MN	X	3035	1/1	0.92	0.21	110,110,110,110	0
32	MN	X	3368	1/1	0.92	0.32	101,101,101,101	0
32	MN	X	3369	1/1	0.92	0.07	85,85,85,85	0
31	MG	X	3057	1/1	0.93	0.39	62,62,62,62	0
32	MN	X	3373	1/1	0.93	0.32	139,139,139,139	0
31	MG	E	201	1/1	0.93	0.26	45,45,45,45	0
32	MN	X	3319	1/1	0.93	0.28	101,101,101,101	0
31	MG	X	3127	1/1	0.93	0.11	46,46,46,46	0
32	MN	X	3323	1/1	0.93	0.30	71,71,71,71	0
32	MN	X	3225	1/1	0.93	0.46	103,103,103,103	0
31	MG	X	3120	1/1	0.93	0.62	66,66,66,66	0
32	MN	X	3388	1/1	0.93	0.13	121,121,121,121	0
34	SPD	X	3431	10/10	0.93	0.37	56,56,56,56	10
34	SPD	X	3432	10/10	0.93	0.28	63,63,63,63	0
32	MN	X	3148	1/1	0.93	0.13	124,124,124,124	0
30	MPD	X	3004	8/8	0.93	0.19	101,101,101,101	0
32	MN	X	3350	1/1	0.93	0.46	139,139,139,139	0
31	MG	X	3053	1/1	0.93	0.24	53,53,53,53	0
32	MN	X	3292	1/1	0.93	0.22	90,90,90,90	0
32	MN	X	3241	1/1	0.93	0.40	85,85,85,85	0
31	MG	X	3187	1/1	0.93	0.58	52,52,52,52	0
31	MG	X	3031	1/1	0.93	0.39	64,64,64,64	0
31	MG	X	3211	1/1	0.93	0.27	44,44,44,44	0
31	MG	X	3042	1/1	0.93	0.19	75,75,75,75	0
32	MN	X	3364	1/1	0.93	0.22	78,78,78,78	0
32	MN	X	3312	1/1	0.93	0.16	50,50,50,50	0
31	MG	X	3044	1/1	0.93	0.20	27,27,27,27	0
32	MN	X	3444	1/1	0.94	0.32	70,70,70,70	0
32	MN	X	3286	1/1	0.94	0.31	50,50,50,50	0
32	MN	X	3236	1/1	0.94	0.41	85,85,85,85	0
32	MN	X	3138	1/1	0.94	0.17	93,93,93,93	0
31	MG	X	3408	1/1	0.94	0.53	62,62,62,62	0
32	MN	X	3084	1/1	0.94	0.49	148,148,148,148	0
32	MN	X	3165	1/1	0.94	0.18	104,104,104,104	0
31	MG	X	3114	1/1	0.94	0.15	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	MN	X	3363	1/1	0.94	0.52	130,130,130,130	0
32	MN	X	3309	1/1	0.94	0.24	77,77,77,77	0
32	MN	X	3310	1/1	0.94	0.29	97,97,97,97	0
32	MN	X	3065	1/1	0.94	0.95	67,67,67,67	1
31	MG	X	3410	1/1	0.94	0.43	49,49,49,49	1
32	MN	X	3370	1/1	0.94	0.37	86,86,86,86	0
32	MN	X	3259	1/1	0.94	0.37	162,162,162,162	0
32	MN	X	3314	1/1	0.94	0.49	116,116,116,116	0
32	MN	X	3067	1/1	0.94	0.57	80,80,80,80	1
32	MN	X	3380	1/1	0.94	0.59	128,128,128,128	0
31	MG	X	3017	1/1	0.94	0.30	53,53,53,53	0
32	MN	X	3208	1/1	0.94	0.28	104,104,104,104	0
31	MG	X	3049	1/1	0.94	0.22	80,80,80,80	0
32	MN	X	3321	1/1	0.94	0.47	116,116,116,116	0
31	MG	X	3113	1/1	0.94	0.23	34,34,34,34	0
32	MN	X	3276	1/1	0.94	0.24	75,75,75,75	0
32	MN	X	3392	1/1	0.94	0.34	137,137,137,137	0
35	EOH	X	3440	3/3	0.94	0.40	53,53,53,53	0
32	MN	X	3332	1/1	0.94	0.54	109,109,109,109	0
32	MN	X	3282	1/1	0.94	0.47	105,105,105,105	0
32	MN	X	3335	1/1	0.94	0.56	67,67,67,67	0
31	MG	X	3407	1/1	0.94	0.15	31,31,31,31	0
35	EOH	K	201	3/3	0.94	0.16	17,17,17,17	0
32	MN	X	3284	1/1	0.94	0.26	58,58,58,58	0
32	MN	X	3285	1/1	0.94	0.40	99,99,99,99	0
31	MG	X	3169	1/1	0.95	0.38	32,32,32,32	0
31	MG	X	3027	1/1	0.95	0.22	38,38,38,38	0
32	MN	X	3150	1/1	0.95	0.35	128,128,128,128	0
32	MN	Y	206	1/1	0.95	0.37	87,87,87,87	0
31	MG	X	3415	1/1	0.95	0.16	38,38,38,38	0
32	MN	X	3037	1/1	0.95	0.17	135,135,135,135	0
32	MN	X	3302	1/1	0.95	0.20	87,87,87,87	0
32	MN	X	3200	1/1	0.95	0.10	77,77,77,77	0
32	MN	X	3243	1/1	0.95	0.16	73,73,73,73	0
32	MN	X	3038	1/1	0.95	0.40	127,127,127,127	0
30	MPD	X	3015	8/8	0.95	0.16	72,72,72,72	0
32	MN	X	3096	1/1	0.95	0.18	144,144,144,144	0
32	MN	X	3206	1/1	0.95	0.34	111,111,111,111	0
32	MN	X	3372	1/1	0.95	0.33	101,101,101,101	0
31	MG	X	3091	1/1	0.95	0.79	69,69,69,69	0
32	MN	X	3256	1/1	0.95	0.31	133,133,133,133	0
32	MN	X	3163	1/1	0.95	0.15	143,143,143,143	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
31	MG	X	3419	1/1	0.95	0.98	57,57,57,57	0
31	MG	X	3128	1/1	0.95	0.21	61,61,61,61	0
32	MN	X	3022	1/1	0.95	0.28	133,133,133,133	0
32	MN	X	3073	1/1	0.95	0.17	140,140,140,140	0
32	MN	X	3074	1/1	0.95	0.16	95,95,95,95	0
32	MN	X	3324	1/1	0.95	0.12	47,47,47,47	0
32	MN	X	3140	1/1	0.95	0.20	82,82,82,82	0
32	MN	X	3390	1/1	0.95	0.30	97,97,97,97	0
32	MN	X	3275	1/1	0.95	0.21	77,77,77,77	0
31	MG	X	3045	1/1	0.95	0.27	65,65,65,65	0
32	MN	X	3281	1/1	0.95	0.26	61,61,61,61	0
32	MN	X	3339	1/1	0.95	0.26	67,67,67,67	0
31	MG	X	3029	1/1	0.95	0.21	55,55,55,55	0
31	MG	X	3030	1/1	0.95	0.71	59,59,59,59	0
32	MN	X	3193	1/1	0.95	0.27	107,107,107,107	0
30	MPD	X	3016	8/8	0.95	0.39	32,32,32,32	0
32	MN	X	3351	1/1	0.96	0.33	117,117,117,117	0
32	MN	X	3402	1/1	0.96	0.31	67,67,67,67	0
32	MN	X	3166	1/1	0.96	0.43	115,115,115,115	0
32	MN	X	3257	1/1	0.96	0.27	110,110,110,110	0
32	MN	X	3405	1/1	0.96	0.35	84,84,84,84	0
32	MN	X	3406	1/1	0.96	0.29	87,87,87,87	0
32	MN	X	3355	1/1	0.96	0.20	115,115,115,115	0
32	MN	X	3306	1/1	0.96	0.32	69,69,69,69	0
31	MG	X	3116	1/1	0.96	0.09	95,95,95,95	0
32	MN	X	3359	1/1	0.96	0.43	125,125,125,125	0
31	MG	X	3059	1/1	0.96	0.23	34,34,34,34	0
32	MN	X	3149	1/1	0.96	0.36	117,117,117,117	0
32	MN	X	3135	1/1	0.96	0.21	114,114,114,114	0
32	MN	X	3263	1/1	0.96	0.32	71,71,71,71	0
32	MN	X	3229	1/1	0.96	0.18	76,76,76,76	0
32	MN	X	3267	1/1	0.96	0.27	74,74,74,74	0
32	MN	X	3151	1/1	0.96	0.17	69,69,69,69	0
32	MN	X	3062	1/1	0.96	0.31	61,61,61,61	0
32	MN	X	3317	1/1	0.96	0.66	112,112,112,112	0
32	MN	X	3371	1/1	0.96	0.32	109,109,109,109	0
32	MN	X	3156	1/1	0.96	0.19	127,127,127,127	0
32	MN	X	3234	1/1	0.96	0.28	70,70,70,70	0
32	MN	X	3064	1/1	0.96	0.05	96,96,96,96	0
32	MN	X	3375	1/1	0.96	0.48	129,129,129,129	0
32	MN	X	3322	1/1	0.96	0.22	52,52,52,52	0
31	MG	C	301	1/1	0.96	0.69	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	MN	X	3214	1/1	0.96	0.31	74,74,74,74	0
32	MN	X	3078	1/1	0.96	0.54	130,130,130,130	0
35	EOH	X	3435	3/3	0.96	0.12	62,62,62,62	0
32	MN	X	3246	1/1	0.96	0.33	86,86,86,86	0
32	MN	X	3384	1/1	0.96	0.17	75,75,75,75	0
31	MG	X	3047	1/1	0.96	0.29	75,75,75,75	0
32	MN	X	3252	1/1	0.96	0.19	127,127,127,127	0
32	MN	X	3131	1/1	0.96	0.44	134,134,134,134	0
32	MN	X	3341	1/1	0.96	0.27	33,33,33,33	0
32	MN	X	3391	1/1	0.96	0.44	132,132,132,132	0
32	MN	X	3343	1/1	0.96	0.33	69,69,69,69	0
32	MN	X	3298	1/1	0.96	0.26	66,66,66,66	0
32	MN	X	3144	1/1	0.96	0.20	116,116,116,116	0
32	MN	X	3396	1/1	0.96	0.09	109,109,109,109	0
31	MG	X	3043	1/1	0.96	0.66	75,75,75,75	0
32	MN	X	3303	1/1	0.97	0.62	118,118,118,118	0
32	MN	X	3353	1/1	0.97	0.53	92,92,92,92	0
32	MN	X	3158	1/1	0.97	0.07	82,82,82,82	0
32	MN	X	3039	1/1	0.97	0.09	153,153,153,153	0
31	MG	X	3094	1/1	0.97	0.29	58,58,58,58	0
32	MN	X	3235	1/1	0.97	0.19	95,95,95,95	0
32	MN	X	3358	1/1	0.97	0.45	122,122,122,122	0
29	3LK	X	3001	40/40	0.97	0.34	31,31,31,31	0
32	MN	X	3238	1/1	0.97	0.29	70,70,70,70	0
32	MN	X	3271	1/1	0.97	0.36	60,60,60,60	0
32	MN	X	3061	1/1	0.97	0.41	68,68,68,68	0
32	MN	X	3242	1/1	0.97	0.16	100,100,100,100	0
32	MN	X	3146	1/1	0.97	0.40	88,88,88,88	0
32	MN	X	3365	1/1	0.97	0.19	69,69,69,69	0
32	MN	X	3279	1/1	0.97	0.34	78,78,78,78	0
32	MN	X	3280	1/1	0.97	0.16	50,50,50,50	0
31	MG	X	3175	1/1	0.97	0.22	17,17,17,17	0
32	MN	X	3245	1/1	0.97	0.32	86,86,86,86	0
32	MN	X	3063	1/1	0.97	0.37	78,78,78,78	0
32	MN	X	3080	1/1	0.97	0.16	111,111,111,111	0
32	MN	X	3221	1/1	0.97	0.38	73,73,73,73	0
31	MG	X	3099	1/1	0.97	0.07	59,59,59,59	0
32	MN	X	3325	1/1	0.97	0.15	62,62,62,62	0
32	MN	X	3326	1/1	0.97	0.18	42,42,42,42	0
32	MN	X	3288	1/1	0.97	0.48	87,87,87,87	0
32	MN	X	3329	1/1	0.97	0.31	53,53,53,53	0
32	MN	X	3289	1/1	0.97	0.20	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
31	MG	B	301	1/1	0.97	0.17	23,23,23,23	0
31	MG	X	3417	1/1	0.97	0.14	45,45,45,45	0
32	MN	X	3337	1/1	0.97	0.28	70,70,70,70	0
32	MN	X	3338	1/1	0.97	0.30	67,67,67,67	0
32	MN	X	3294	1/1	0.97	0.16	47,47,47,47	0
32	MN	X	3340	1/1	0.97	0.32	23,23,23,23	0
32	MN	X	3295	1/1	0.97	0.17	55,55,55,55	0
32	MN	X	3296	1/1	0.97	0.32	78,78,78,78	0
31	MG	X	3100	1/1	0.97	0.22	95,95,95,95	0
32	MN	X	3347	1/1	0.97	0.18	106,106,106,106	0
32	MN	X	3189	1/1	0.97	0.19	138,138,138,138	0
32	MN	X	3207	1/1	0.97	0.14	94,94,94,94	0
31	MG	X	3170	1/1	0.97	0.15	60,60,60,60	0
31	MG	X	3106	1/1	0.98	0.49	28,28,28,28	1
32	MN	X	3398	1/1	0.98	0.22	88,88,88,88	0
32	MN	X	3274	1/1	0.98	0.26	37,37,37,37	0
32	MN	X	3400	1/1	0.98	0.06	106,106,106,106	0
32	MN	X	3401	1/1	0.98	0.31	67,67,67,67	0
32	MN	X	3164	1/1	0.98	0.22	104,104,104,104	0
32	MN	X	3083	1/1	0.98	0.45	44,44,44,44	0
32	MN	X	3278	1/1	0.98	0.21	55,55,55,55	0
32	MN	X	3247	1/1	0.98	0.35	48,48,48,48	0
32	MN	X	3248	1/1	0.98	0.51	71,71,71,71	0
32	MN	X	3155	1/1	0.98	0.21	89,89,89,89	0
32	MN	X	3251	1/1	0.98	0.19	131,131,131,131	0
32	MN	X	3178	1/1	0.98	0.21	88,88,88,88	0
31	MG	X	3172	1/1	0.98	0.43	36,36,36,36	0
32	MN	X	3136	1/1	0.98	0.21	84,84,84,84	0
32	MN	X	3213	1/1	0.98	0.18	72,72,72,72	0
32	MN	X	3137	1/1	0.98	0.43	110,110,110,110	0
32	MN	X	3366	1/1	0.98	0.17	71,71,71,71	0
32	MN	X	3097	1/1	0.98	0.25	108,108,108,108	0
32	MN	X	3024	1/1	0.98	0.12	150,150,150,150	0
32	MN	X	3217	1/1	0.98	0.41	92,92,92,92	0
32	MN	X	3293	1/1	0.98	0.21	29,29,29,29	0
32	MN	X	3328	1/1	0.98	0.17	48,48,48,48	0
32	MN	X	3237	1/1	0.98	0.22	66,66,66,66	0
32	MN	X	3331	1/1	0.98	0.27	94,94,94,94	0
32	MN	X	3201	1/1	0.98	0.11	85,85,85,85	0
32	MN	X	3239	1/1	0.98	0.20	55,55,55,55	0
32	MN	X	3376	1/1	0.98	0.26	57,57,57,57	0
32	MN	X	3334	1/1	0.98	0.23	48,48,48,48	0

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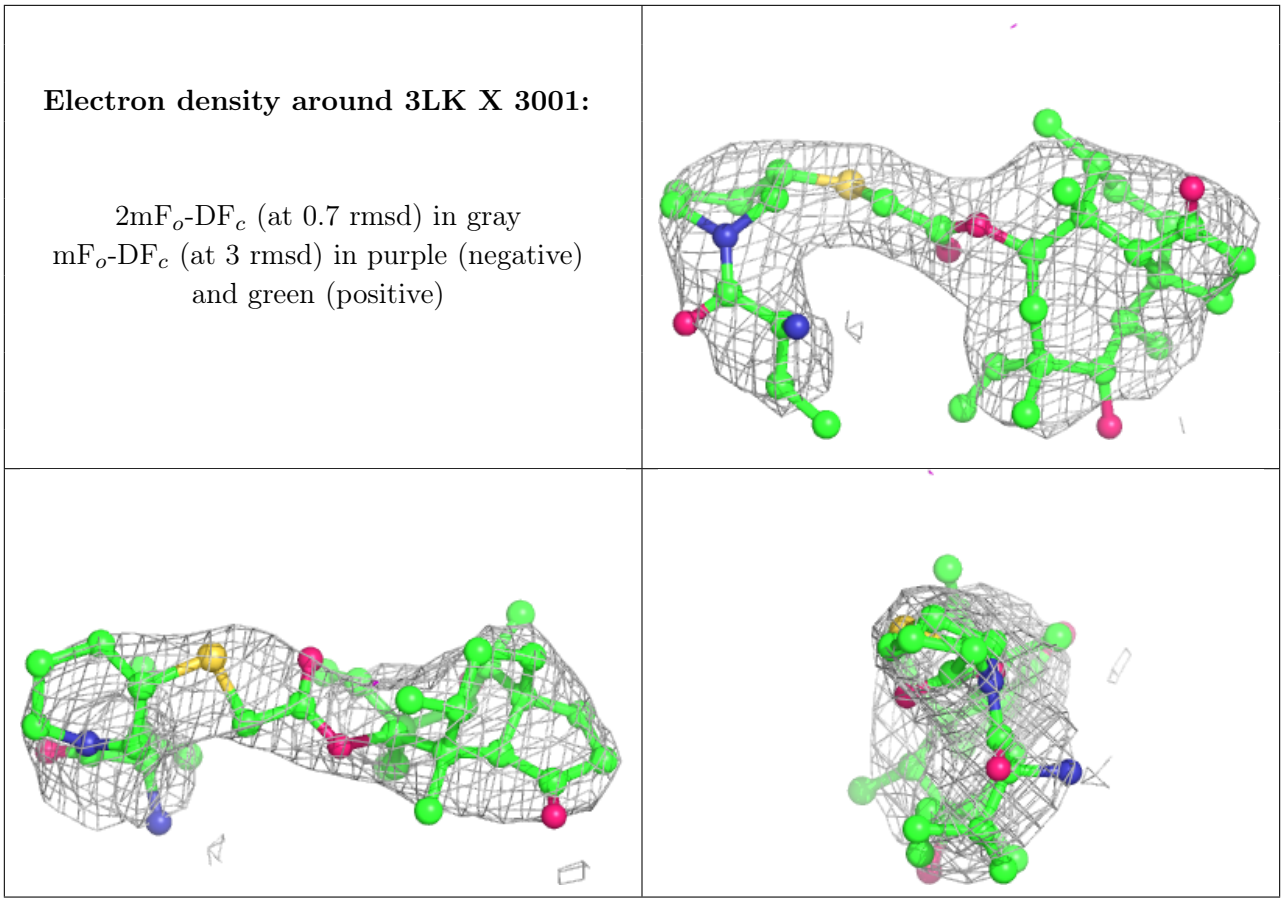
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	MN	X	3379	1/1	0.98	0.34	98,98,98,98	0
32	MN	X	3297	1/1	0.98	0.27	52,52,52,52	0
32	MN	X	3336	1/1	0.98	0.42	48,48,48,48	0
32	MN	X	3240	1/1	0.98	0.19	73,73,73,73	0
32	MN	X	3299	1/1	0.98	0.17	69,69,69,69	0
32	MN	X	3266	1/1	0.98	0.52	83,83,83,83	0
32	MN	X	3068	1/1	0.98	0.28	34,34,34,34	0
32	MN	X	3268	1/1	0.98	0.34	73,73,73,73	0
32	MN	X	3087	1/1	0.98	0.24	120,120,120,120	0
32	MN	X	3345	1/1	0.98	0.35	54,54,54,54	0
32	MN	X	3270	1/1	0.98	0.37	60,60,60,60	0
32	MN	X	3305	1/1	0.98	0.32	80,80,80,80	0
32	MN	X	3393	1/1	0.98	0.39	80,80,80,80	0
32	MN	X	3204	1/1	0.98	0.19	78,78,78,78	0
32	MN	X	3307	1/1	0.98	0.26	78,78,78,78	0
32	MN	X	3272	1/1	0.98	0.38	43,43,43,43	0
32	MN	X	3342	1/1	0.99	0.49	49,49,49,49	0
32	MN	X	3287	1/1	0.99	0.27	57,57,57,57	0
32	MN	X	3344	1/1	0.99	0.32	46,46,46,46	0
32	MN	X	3153	1/1	0.99	0.10	66,66,66,66	0
32	MN	X	3265	1/1	0.99	0.33	60,60,60,60	0
32	MN	X	3330	1/1	0.99	0.20	55,55,55,55	0
32	MN	X	3348	1/1	0.99	0.20	32,32,32,32	0
32	MN	X	3386	1/1	0.99	0.31	65,65,65,65	0
32	MN	X	3387	1/1	0.99	0.12	59,59,59,59	0
32	MN	X	3290	1/1	0.99	0.27	66,66,66,66	0
31	MG	X	3174	1/1	0.99	0.51	55,55,55,55	0
32	MN	X	3318	1/1	0.99	0.20	57,57,57,57	0
31	MG	X	3420	1/1	0.99	0.64	30,30,30,30	0
32	MN	X	3232	1/1	0.99	0.19	84,84,84,84	0
32	MN	X	3081	1/1	0.99	0.32	32,32,32,32	0
32	MN	X	3250	1/1	0.99	0.06	66,66,66,66	0
31	MG	Y	201	1/1	0.99	0.18	83,83,83,83	0
32	MN	X	3072	1/1	0.99	0.23	38,38,38,38	0
32	MN	X	3262	1/1	0.99	0.30	59,59,59,59	0
32	MN	X	3377	1/1	0.99	0.26	55,55,55,55	0
31	MG	X	3227	1/1	0.99	0.19	35,35,35,35	0
32	MN	X	3154	1/1	1.00	0.18	75,75,75,75	0
32	MN	X	3277	1/1	1.00	0.21	35,35,35,35	0

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

orientation to approximate a three-dimensional view.

Electron density around 3LK X 3001:

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



6.5 Other polymers

There are no such residues in this entry.