wwPDB X-ray Structure Validation Summary Report (i)

Jan 2, 2024 – 10:07 am GMT

PDB ID	:	5HL7
Title	:	The crystal structure of the large ribosomal subunit of Staphylococcus aureus in complex with lefamulin
Authors	:	Eyal, Z.; Matzov, D.; Krupkin, M.; Rozenberg, H.; Zimmerman, E.; Bashan, A.; Yonath, A.
Deposited on	:	2016-01-14
Resolution	:	3.55 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:

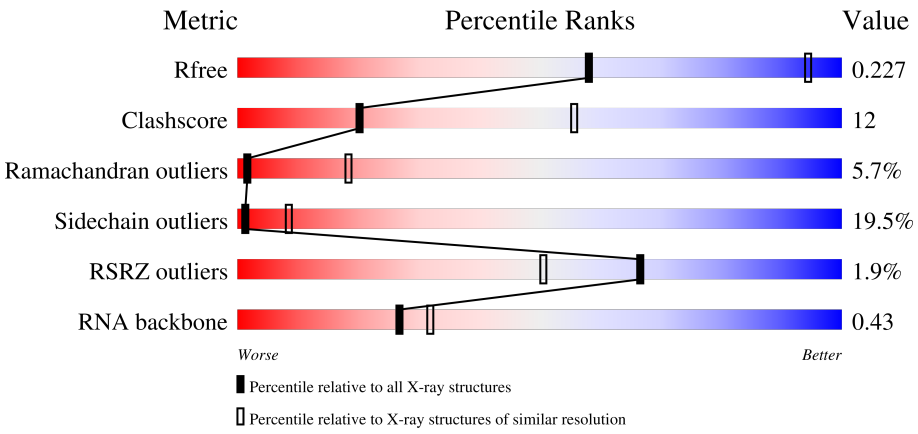
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)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

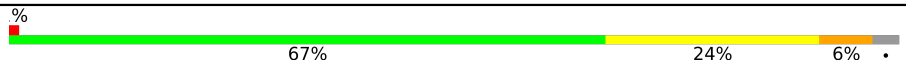
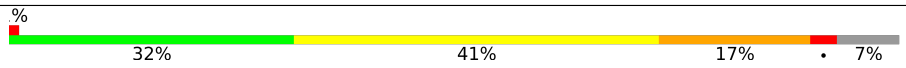
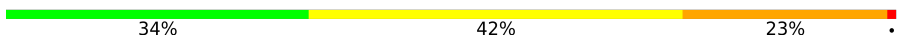
The reported resolution of this entry is 3.55 Å.

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	1020 (3.62-3.50)
Clashscore	141614	1100 (3.62-3.50)
Ramachandran outliers	138981	1065 (3.62-3.50)
Sidechain outliers	138945	1066 (3.62-3.50)
RSRZ outliers	127900	1009 (3.64-3.48)
RNA backbone	3102	1008 (4.10-3.00)

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 <=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	A	277	
2	X	2923	
3	Y	114	

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Mol	Chain	Length	Quality of chain
4	B	220	55% 34% 9%
5	C	207	53% 34% 9%
6	D	179	6% 78% 13% 8%
7	E	178	3% 65% 19% 5% 12%
8	G	145	% 54% 36% 10%
9	H	122	52% 38% 10%
10	I	140	4% 57% 24% 12% 6%
11	J	144	3% 60% 32%
12	K	122	51% 42%
13	L	119	67% 18% 6% 8%
14	M	116	2% 54% 28% 12% 5%
15	N	118	51% 41% 7%
16	O	102	62% 33% 5%
17	P	117	% 57% 33% 5%
18	Q	91	62% 32% 5%
19	R	105	6% 51% 29% 17%
20	S	217	47% 23% 6% 23%
21	T	94	% 48% 23% 9% 20%
22	U	62	39% 55% 11% 32%
23	V	69	49% 42% 6%
24	W	59	42% 39% 14%
25	Z	58	41% 28% 5% 26%
26	2	45	9% 56% 33% 7%
27	3	66	50% 30% 11% 9%
28	4	37	59% 78% 19%

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
29	MN	X	3114	-	-	-	X
29	MN	X	3155	-	-	-	X
29	MN	X	3186	-	-	-	X
29	MN	X	3225	-	-	-	X
29	MN	X	3421	-	-	-	X
29	MN	X	3446	-	-	-	X
29	MN	X	3454	-	-	-	X
29	MN	X	3458	-	-	-	X
29	MN	X	3471	-	-	-	X
30	MG	A	302	-	-	-	X
30	MG	G	201	-	-	-	X
30	MG	P	201	-	-	-	X
30	MG	X	3087	-	-	-	X
30	MG	X	3180	-	-	-	X
30	MG	X	3196	-	-	-	X
30	MG	X	3230	-	-	-	X
30	MG	X	3236	-	-	-	X
30	MG	X	3244	-	-	-	X
30	MG	X	3248	-	-	-	X
30	MG	X	3250	-	-	-	X
30	MG	X	3252	-	-	-	X
30	MG	X	3253	-	-	-	X
30	MG	X	3254	-	-	-	X
30	MG	X	3255	-	-	-	X
30	MG	X	3265	-	-	-	X
30	MG	X	3286	-	-	-	X
30	MG	X	3293	-	-	-	X
30	MG	X	3294	-	-	-	X
30	MG	X	3306	-	-	-	X
30	MG	X	3308	-	-	-	X
30	MG	X	3327	-	-	-	X
30	MG	X	3332	-	-	-	X
30	MG	X	3335	-	-	-	X
30	MG	X	3336	-	-	-	X
30	MG	X	3337	-	-	-	X
30	MG	X	3339	-	-	-	X
30	MG	X	3340	-	-	-	X
30	MG	X	3341	-	-	-	X
30	MG	X	3342	-	-	-	X
30	MG	X	3344	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	MG	X	3346	-	-	-	X
30	MG	X	3348	-	-	-	X
30	MG	X	3349	-	-	-	X
30	MG	X	3351	-	-	-	X
30	MG	X	3352	-	-	-	X
30	MG	X	3358	-	-	-	X
30	MG	X	3365	-	-	-	X
30	MG	X	3370	-	-	-	X
30	MG	X	3382	-	-	-	X
30	MG	X	3386	-	-	-	X
30	MG	X	3391	-	-	-	X
30	MG	X	3393	-	-	-	X
30	MG	X	3398	-	-	-	X
30	MG	X	3400	-	-	-	X
30	MG	X	3413	-	-	-	X
30	MG	X	3417	-	-	-	X
30	MG	X	3441	-	-	-	X
30	MG	X	3445	-	-	-	X
30	MG	X	3449	-	-	-	X
30	MG	X	3475	-	-	-	X
30	MG	X	3487	-	-	-	X
30	MG	X	3488	-	-	-	X
30	MG	Y	203	-	-	-	X
30	MG	Y	210	-	-	-	X
30	MG	Y	212	-	-	-	X
33	SPD	X	3498	-	-	-	X
35	EPE	N	201	-	-	X	-

2 Entry composition (i)

There are 35 unique types of molecules in this entry. The entry contains 81462 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 protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	269	1667	1007	331	324	5	0	0	0

- Molecule 2 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	X	2705	57983	25884	10620	18774	2705	0	0	0

- Molecule 3 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	Y	114	2430	1086	436	794	114	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	967	289	286	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	1324	823	250	249	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	165	853	512	165	174	2	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	157	915	559	172	182	2	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	174	LYS	GLY	conflict	UNP Q2FW21

- 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	1090	682	202	203	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	884	548	167	165	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	819	498	164	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	138	1001	641	187	170	3	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	906	556	175	174	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	109	673	411	134	128	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	110	807	510	162	135	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	922	581	183	154	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	S			
16	O	102	751	477	138	135	1	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	112	853	531	161	158	3	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	90	583	365	103	112	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	102	627	382	120	124	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	167	1087	682	191	212	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	559	349	110	100	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	42	242	149	48	45	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	486	299	89	98	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	437	271	82	84	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	43	339	208	70	57	4	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	43	350	213	85	51	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	248	81	74	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	36	181	107	36	36	2	0	0	0

- Molecule 29 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mn		
29	A	1	1	1	0	0
29	X	268	Total 268	Mn 268	0	0
29	Y	2	Total 2	Mn 2	0	0
29	R	1	Total 1	Mn 1	0	0
29	T	1	Total 1	Mn 1	0	0
29	Z	1	Total 1	Mn 1	0	0

- Molecule 30 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
30	A	3	3	3	0	0
30	X	218	Total 218	Mg 218	0	0
30	Y	10	Total 10	Mg 10	0	0
30	C	2	Total 2	Mg 2	0	0
30	G	2	Total 2	Mg 2	0	0
30	I	1	Total 1	Mg 1	0	0
30	J	1	Total 1	Mg 1	0	0

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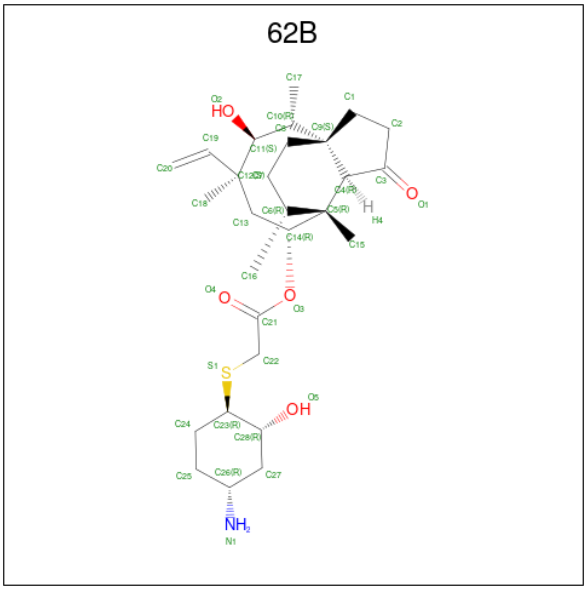
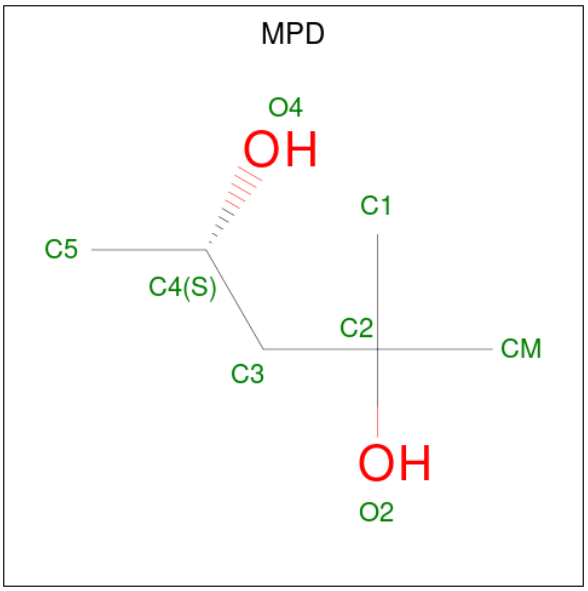
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
30	M	1	1	1	0	0
			Total	Mg		
30	O	1	1	1	0	0
			Total	Mg		
30	P	1	1	1	0	0

- Molecule 31 is Lefamulin (three-letter code: 62B) (formula: $C_{28}H_{45}NO_5S$).



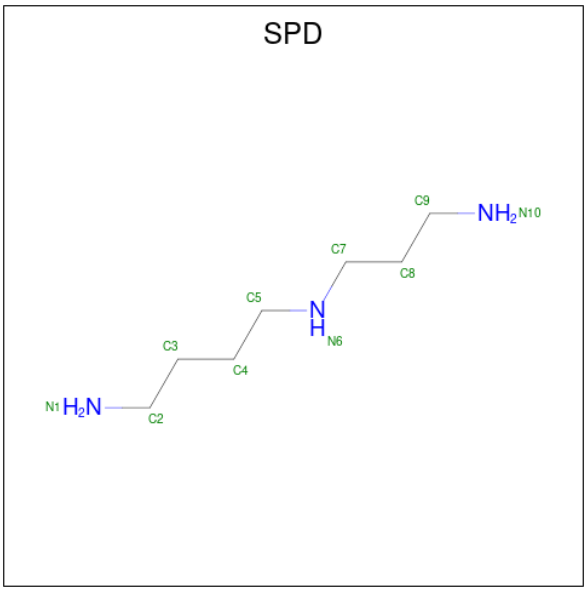
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
31	X	1	35	28	1	5	1	0	0

- Molecule 32 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



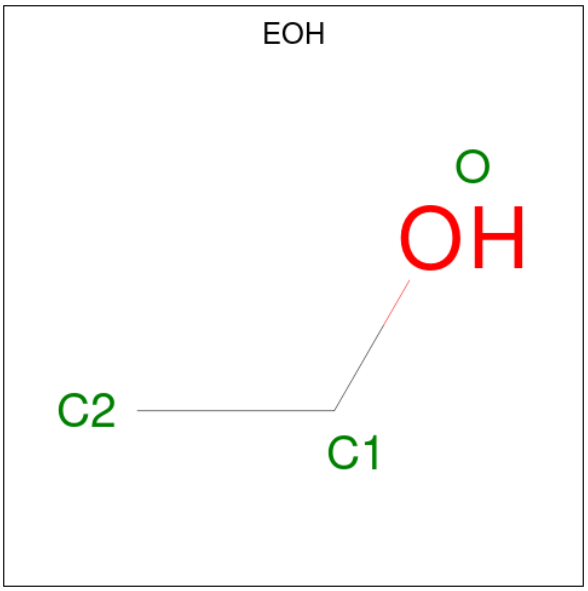
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	X	1	Total	C	O		0	0
			8	6	2			
32	X	1	Total	C	O		0	0
			8	6	2			
32	X	1	Total	C	O		0	0
			8	6	2			
32	X	1	Total	C	O		0	0
			8	6	2			
32	X	1	Total	C	O		0	0
			8	6	2			
32	X	1	Total	C	O		0	0
			8	6	2			
32	X	1	Total	C	O		0	0
			8	6	2			
32	X	1	Total	C	O		0	0
			8	6	2			
32	J	1	Total	C	O		0	0
			8	6	2			
32	Q	1	Total	C	O		0	0
			8	6	2			
32	Z	1	Total	C	O		0	0
			8	6	2			

- Molecule 33 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



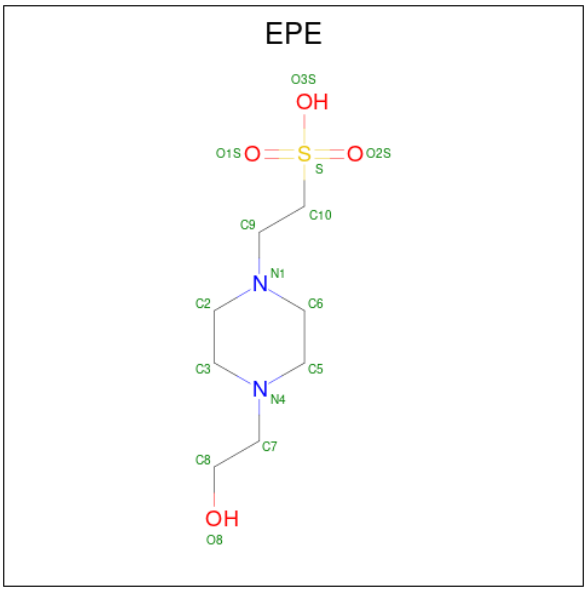
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	X	1	Total	C	N		0	0
			10	7	3			
33	X	1	Total	C	N		0	0
			10	7	3			
33	X	1	Total	C	N		0	0
			10	7	3			
33	X	1	Total	C	N		0	0
			10	7	3			
33	X	1	Total	C	N		0	0
			10	7	3			
33	X	1	Total	C	N		0	0
			10	7	3			
33	X	1	Total	C	N		0	0
			10	7	3			
33	Y	1	Total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

- Molecule 34 is ETHANOL (three-letter code: EOH) (formula: C_2H_6O).



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

- Molecule 35 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



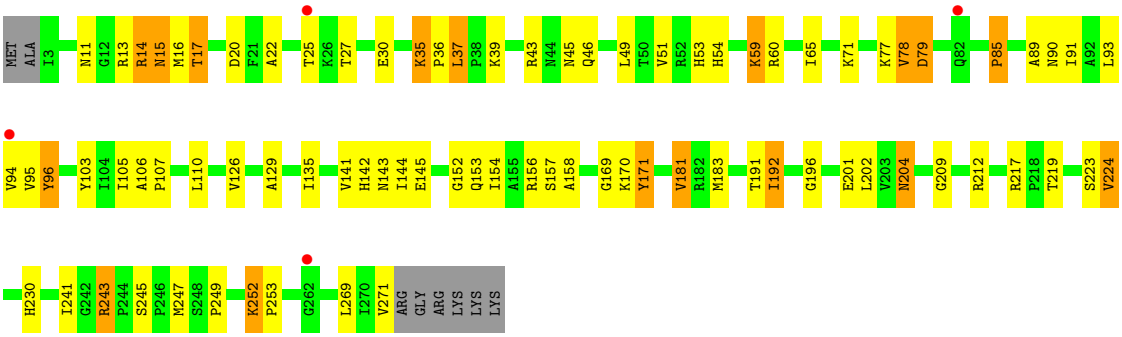
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
35	N	1	15	8	2	4	1	0	0

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.

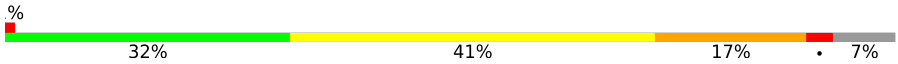
- Molecule 1: 50S ribosomal protein L2

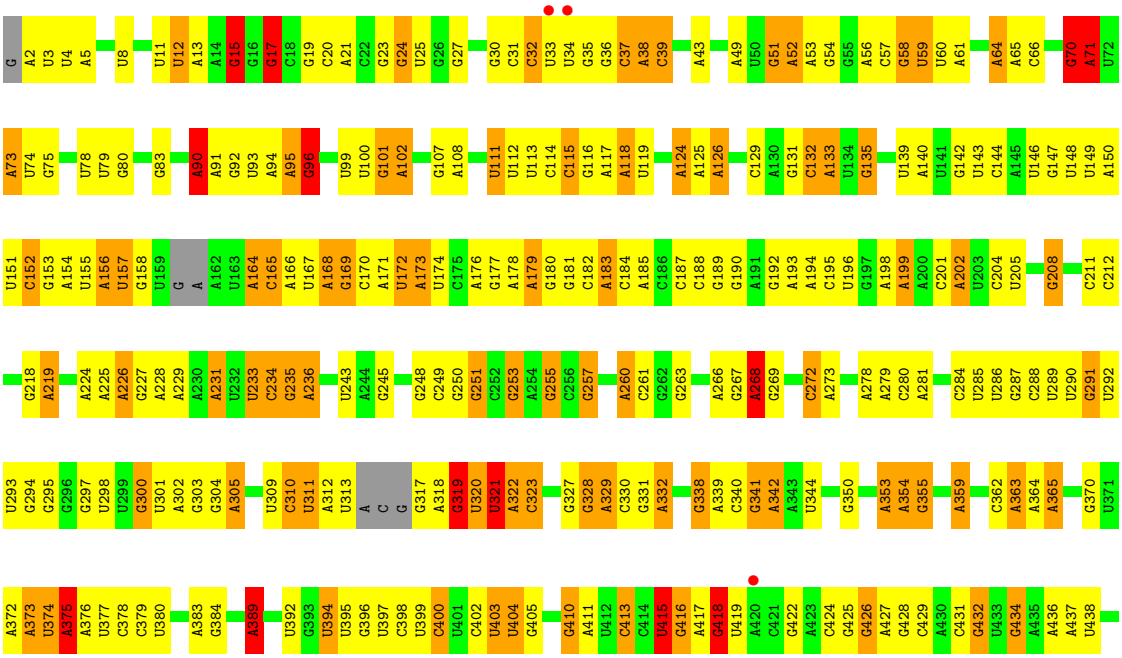
Chain A:

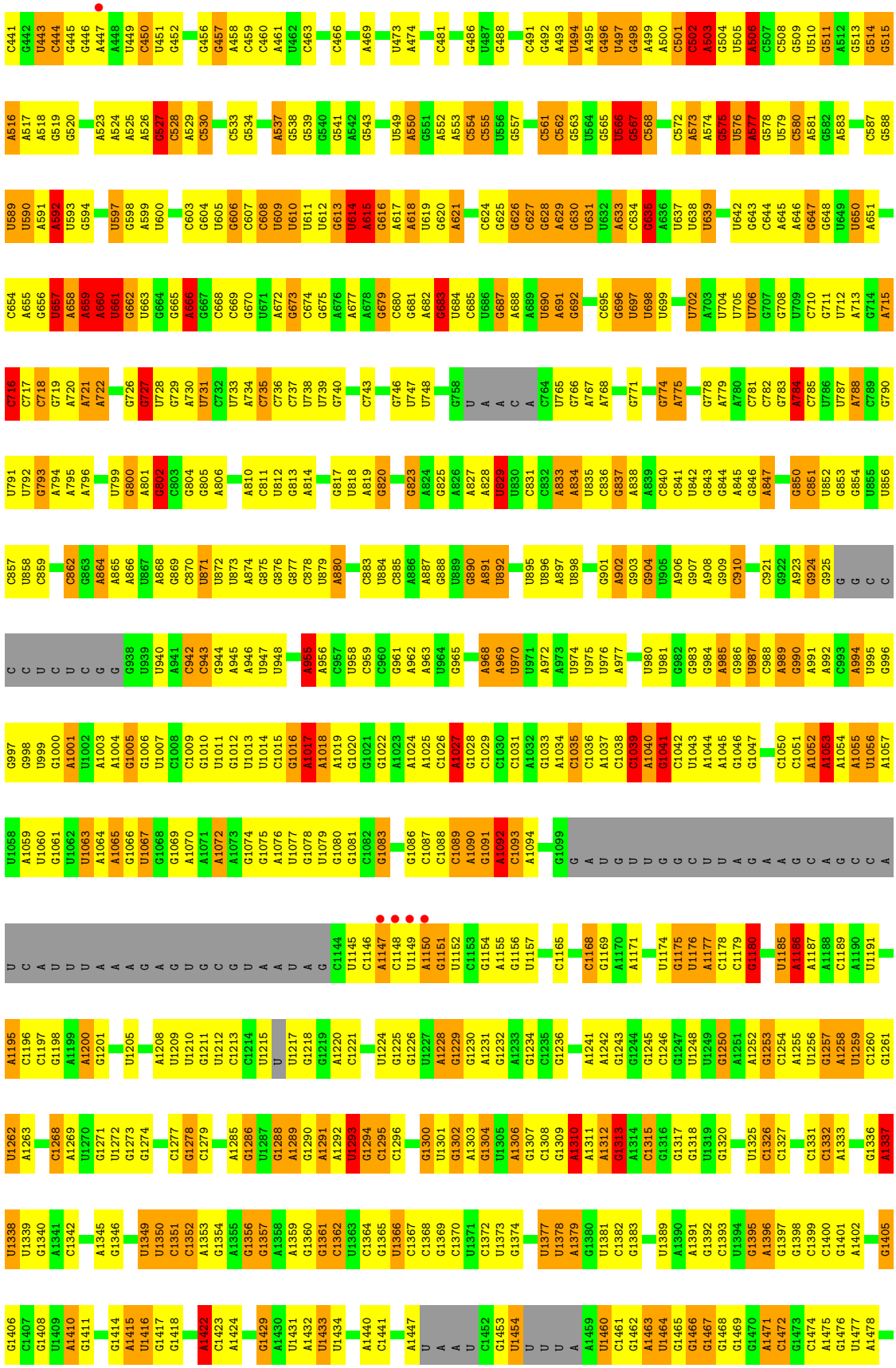


- Molecule 2: 23S ribosomal RNA

Chain X:



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A516 A517 A518 G519 G520 A523 A524 A525 A526 G527 C528 A529 C530 C533 G534 A537 G538 G539 G540 G541 A542 G543 U549 A550 G551 A552 A553 C554 C555 U556 G557 C561 C562 G563 U564 G565 U566 G567 C568 C572 A573 A574 G575 U576 A577 G578 U579 C580 A581 G582 A583 C587 G588
U589 U590 A591 A592 U593 G594 U597 G598 A599 U600 C603 G604 U605 G606 C607 C608 U609 U610 U611 U612 G613 U614 A615 G616 A617 A618 U619 G620 A621 C624 G625 G626 C627 G628 A629 G630 U631 U632 A633 C634 G635 A636 U637 U638 U639 U642 G643 C644 A645 A646 G647 G648 U649 U650 A651
C654 A655 G656 U657 A658 A659 A660 U661 G662 U663 G664 G665 A666 G667 C668 C669 G670 U671 A672 G673 C674 G675 A676 A677 A678 G679 C680 G681 A682 G683 U684 C685 U686 G687 A688 A689 U690 A691 G692 C695 G696 U697 U698 U699 U702 A703 U704 U705 U706 G707 G708 U709 C710 G711 U712 A713 G714 A715
C716 C717 C718 G719 A720 A721 A722 G726 G727 U728 G729 A730 U731 C732 U733 A734 C735 C736 C737 U738 U739 G740 C743 G746 U747 U748 G758 U A A C A C764 U765 G766 A767 A768 G771 G774 A775 G778 A779 A780 C781 C782 G783 A784 C785 U786 U787 A788 C789 G790
U791 U792 G793 A794 A795 A796 U799 G800 A801 G802 C803 G804 G805 A806 A810 C811 U812 G813 A814 G817 U818 A819 G820 G823 A824 G825 A826 A827 A828 U829 U830 C831 C832 A833 A834 U835 C836 G837 A838 A839 C840 C841 U842 G843 G844 A845 G846 A847 G850 C851 U852 G853 G854 U855 U856
C857 U858 C859 C862 G863 A864 A865 A866 U867 A868 G869 C870 U871 U872 U873 A874 G875 G876 G877 C878 U879 A880 C883 U884 C885 A886 A887 G888 U889 G890 A891 U892 U895 U896 A897 U898 G901 A902 G903 G904 U905 A906 G907 A908 G909 C910 C921 G922 A923 G924 G925 G G C C
C C U C U C G G G938 U939 U940 A941 C942 C943 G944 A945 A946 U947 U948 A955 A956 C957 U958 C959 C960 G961 A962 A963 U964 G965 A968 A969 U970 U971 A972 A973 U974 U975 U976 A977 U980 U981 G982 G983 G984 A985 G986 U987 C988 A989 G990 A991 A992 G993 A994 U995 G996
G997 G998 U999 G1000 A1001 U1002 A1003 A1004 G1005 G1006 U1007 G1008 C1009 G1010 U1011 G1012 U1013 U1014 C1015 G1016 A1017 A1018 A1019 G1020 G1021 C1022 A1023 A1024 A1025 C1026 A1027 G1028 C1029 C1030 C1031 A1032 G1033 A1034 C1035 C1036 A1037 C1038 C1039 A1040 G1041 C1042 U1043 A1044 A1045 G1046 G1047 C1050 C1051 A1052 A1053 A1054 A1055 U1056 A1057
U1058 A1059 U1060 G1061 U1062 U1063 A1064 A1065 G1066 U1067 G1068 G1069 A1070 A1071 A1072 A1073 G1074 G1075 A1076 U1077 G1078 U1079 G1080 G1081 C1082 G1083 G1086 C1087 C1088 C1089 A1090 G1091 A1092 C1093 A1094 G1099 G A U G U U G G C U U C A G A G C A A U A
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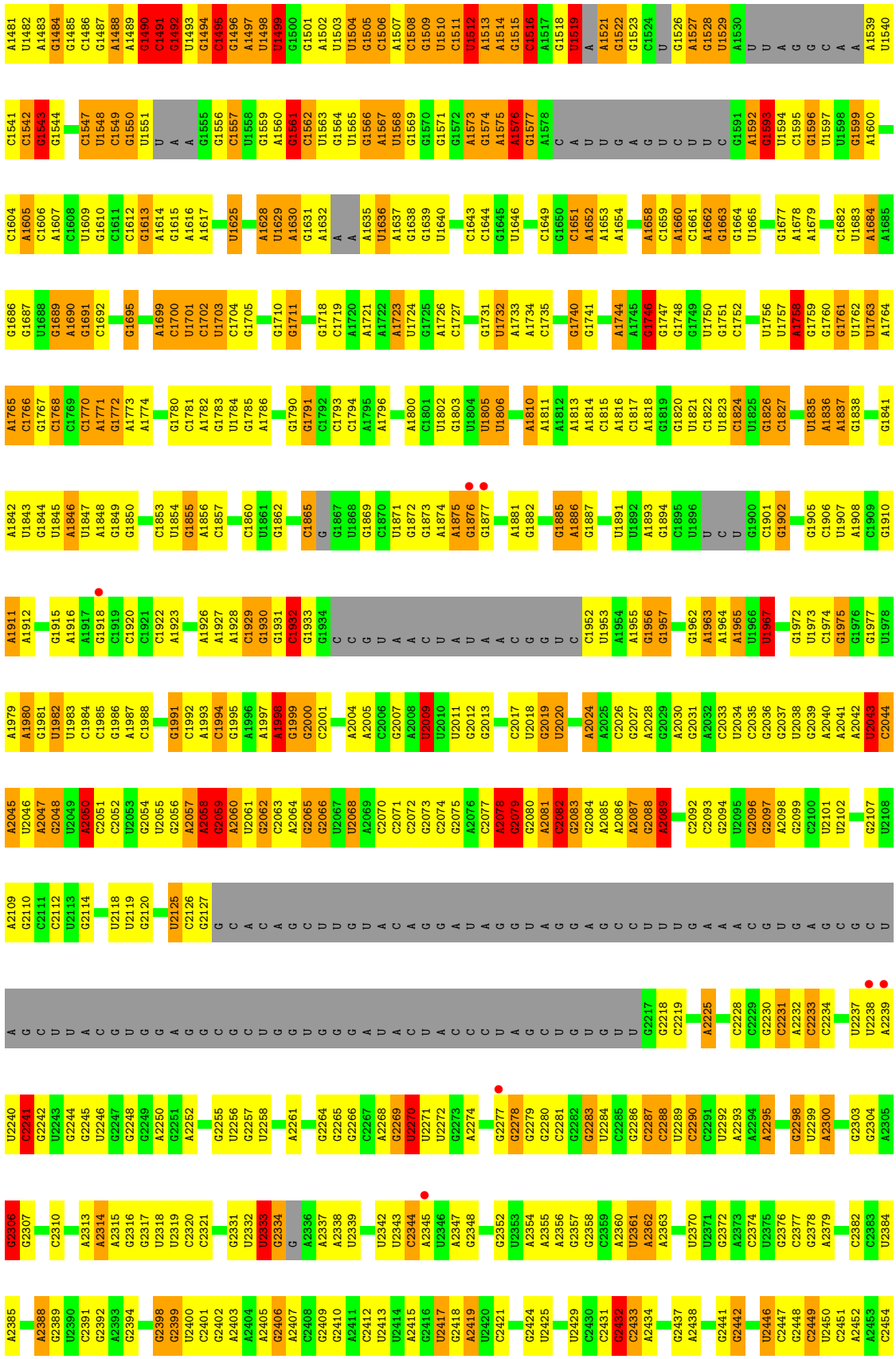
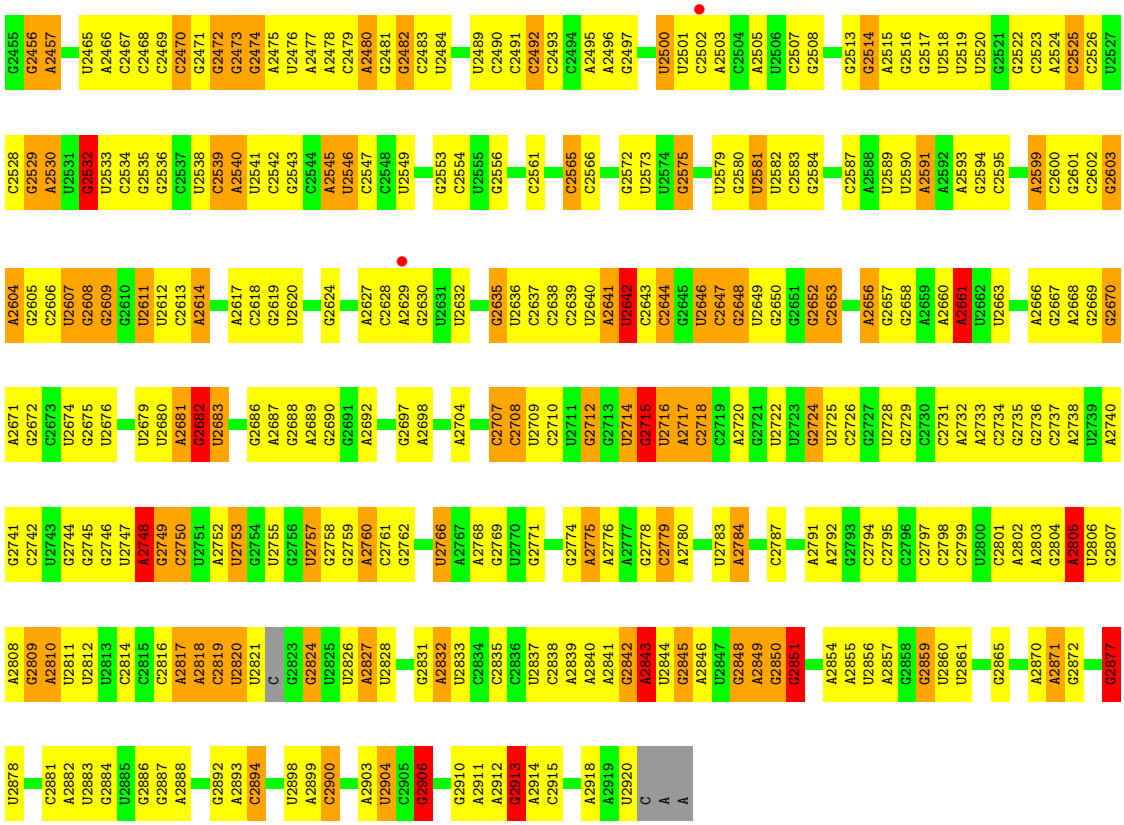
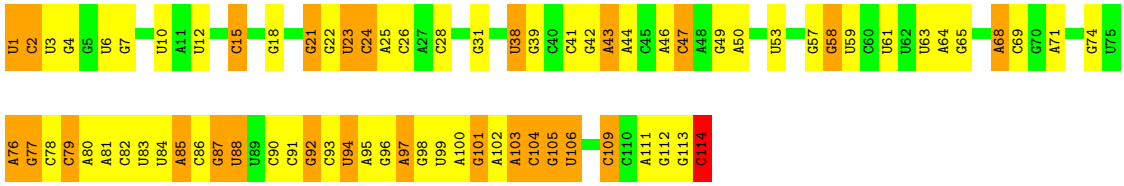
U1262 A1263 C1268 A1269 U1270 G1271 U1272 G1273 G1274 C1277 G1278 C1279 A1285 G1286 U1287 G1288 A1289 G1290 A1291 A1292 U1293 G1294 C1295 U1296 G1300 U1301 G1302 A1303 G1304 U1305 A1306 G1307 C1308 G1309 A1310 A1311 A1312 G1313 A1314 C1315 G1316 G1317 G1318 U1319 G1320 U1325 C1326 C1327 C1331 C1332 A1333 G1336 A1337
U1338 U1339 G1340 A1341 C1342 A1345 G1346 U1349 U1350 C1351 C1352 A1353 G1354 A1355 G1356 G1357 A1358 A1359 G1360 G1361 C1362 U1363 C1364 G1365 U1366 C1367 C1368 G1369 C1370 U1371 C1372 U1373 G1374 U1377 U1378 A1379 G1380 U1381 C1382 G1383 U1389 A1390 A1391 G1392 C1393 U1394 G1395 A1396 G1397 G1398 C1399 C1400 G1401 A1402 G1405
G1406 C1407 G1408 U1409 A1410 G1411 G1414 A1415 U1416 G1417 G1418 A1422 C1423 A1424 G1429 A1430 A1431 A1432 U1433 C1434 A1440 C1441 A1447 U C A U C1452 G1453 U1454 U U U A A1459 U1460 C1461 G1462 A1463 U1464 G1465 G1466 G1467 G1468 G1469 G1470 A1471 C1472 G1473 C1474 A1475 G1476 U1477 A1478





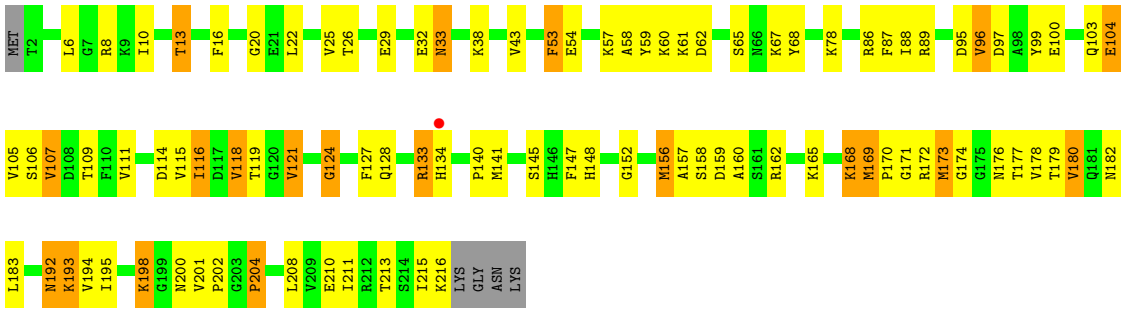
• Molecule 3: 5S ribosomal RNA

Chain Y:



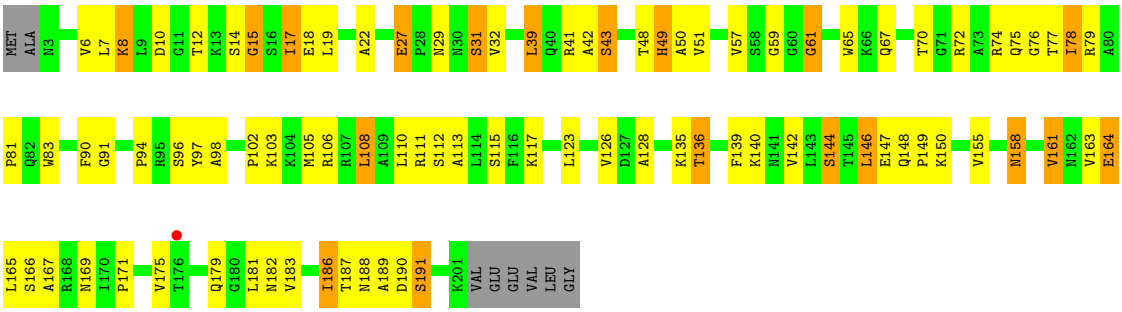
• Molecule 4: 50S ribosomal protein L3

Chain B:



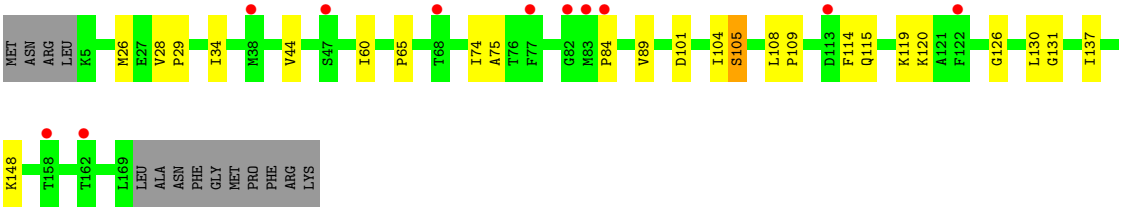
• Molecule 5: 50S ribosomal protein L4

Chain C:



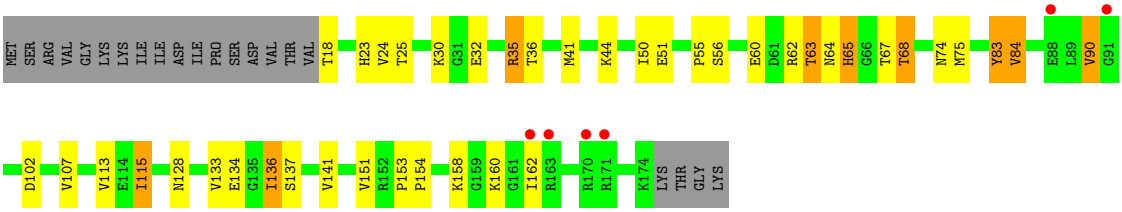
- Molecule 6: 50S ribosomal protein L5

Chain D:



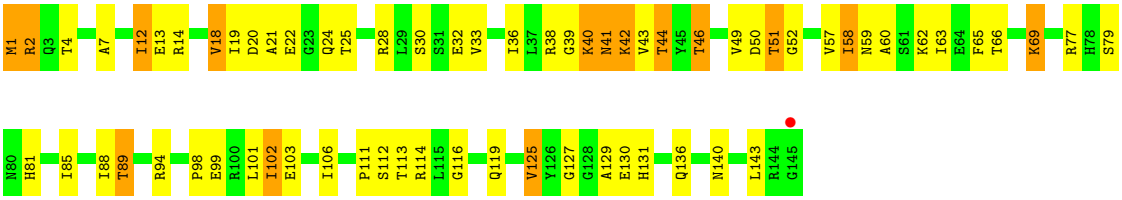
- Molecule 7: 50S ribosomal protein L6

Chain E:



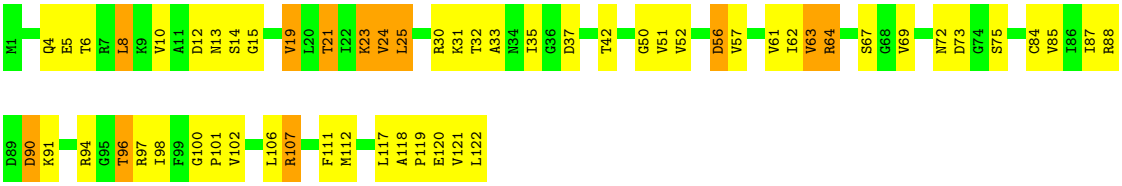
- Molecule 8: 50S ribosomal protein L13

Chain G:



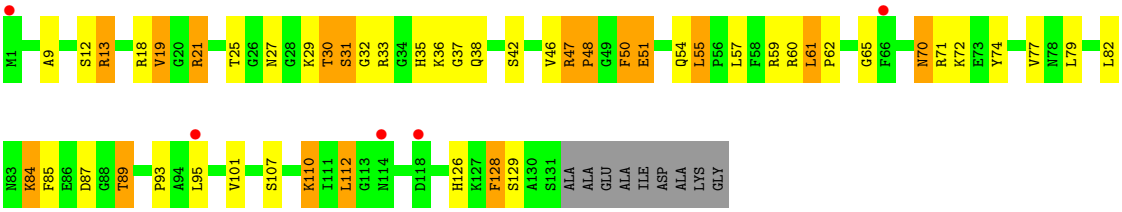
- Molecule 9: 50S ribosomal protein L14

Chain H:



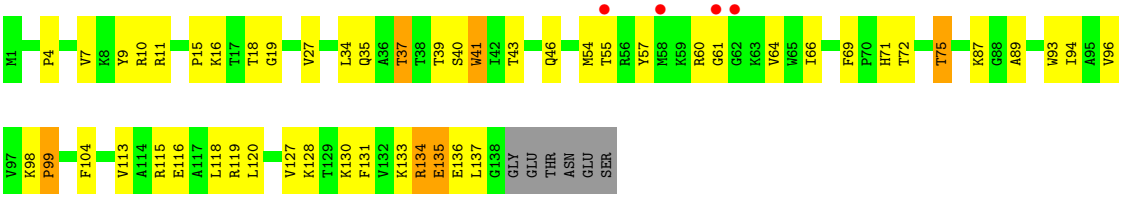
• Molecule 10: 50S ribosomal protein L15

Chain I:



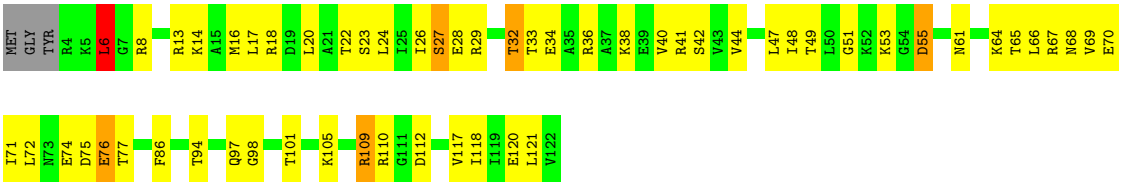
• Molecule 11: 50S ribosomal protein L16

Chain J:



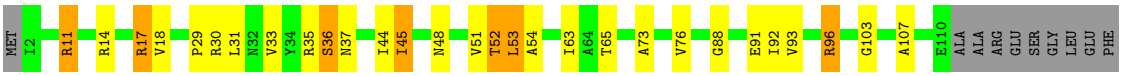
• Molecule 12: 50S ribosomal protein L17

Chain K:



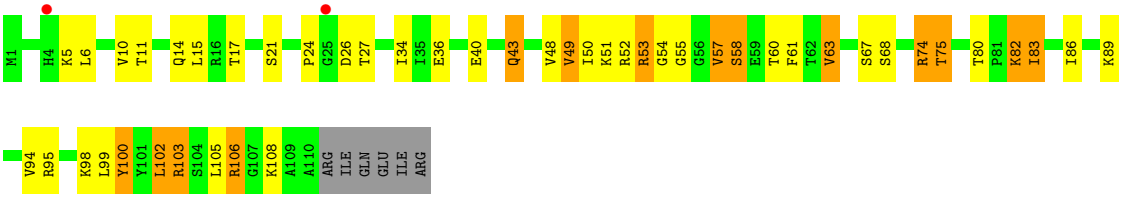
• Molecule 13: 50S ribosomal protein L18

Chain L:



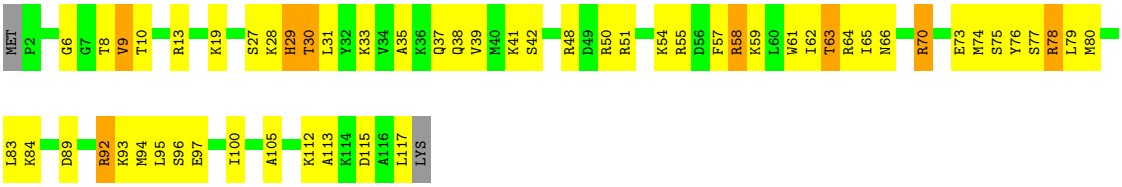
• Molecule 14: 50S ribosomal protein L19

Chain M:



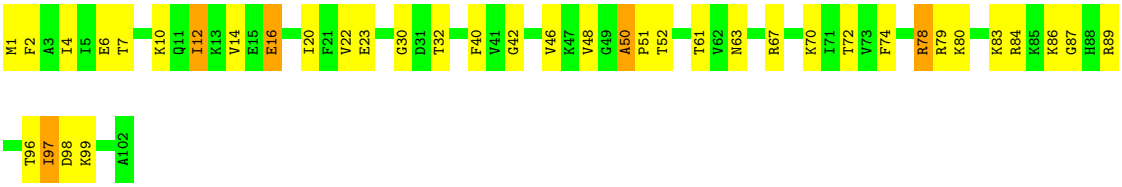
- Molecule 15: 50S ribosomal protein L20

Chain N:



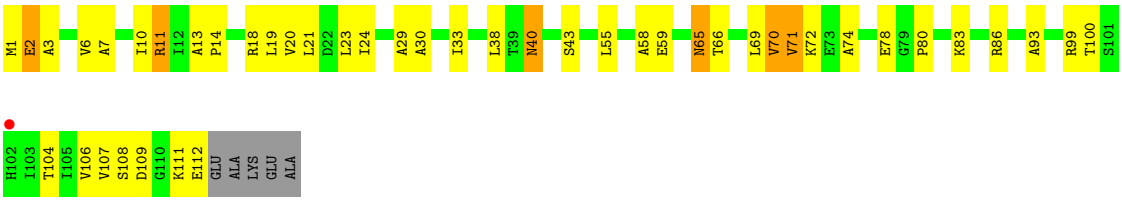
- Molecule 16: 50S ribosomal protein L21

Chain O:



- Molecule 17: 50S ribosomal protein L22

Chain P:

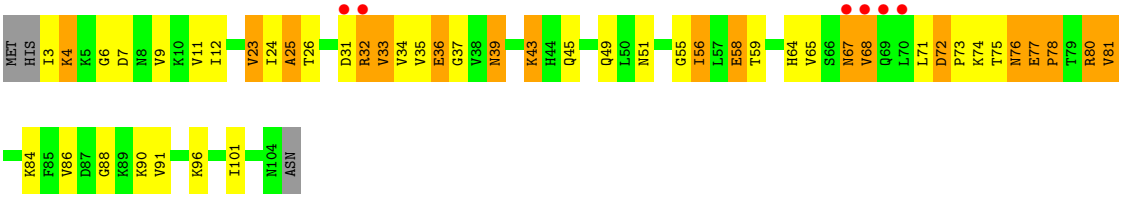


- Molecule 18: 50S ribosomal protein L23

Chain Q:

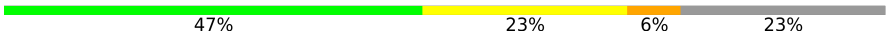
- Molecule 19: 50S ribosomal protein L24

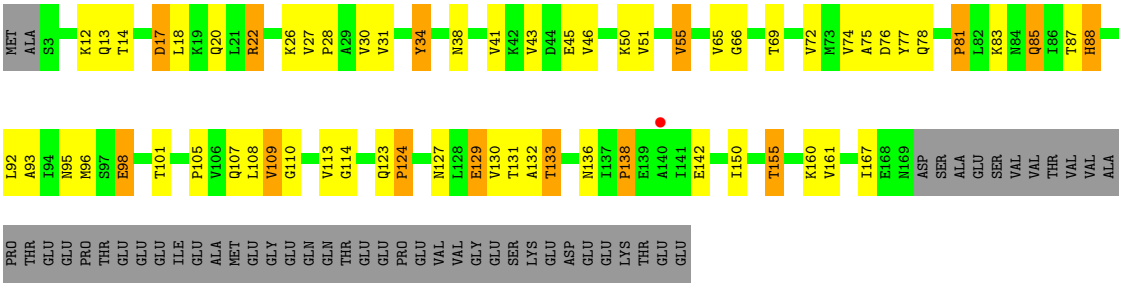
Chain R:



- Molecule 20: 50S ribosomal protein L25

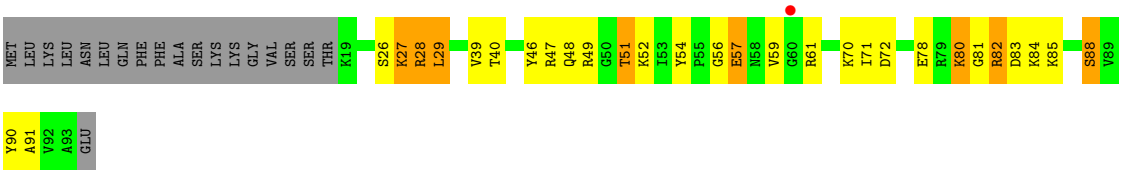
Chain S:





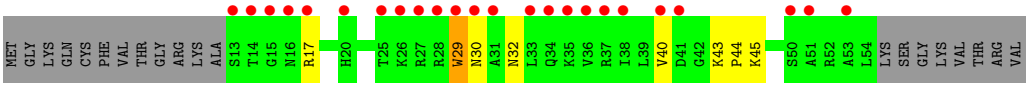
- Molecule 21: 50S ribosomal protein L27

Chain T:



- Molecule 22: 50S ribosomal protein L28

Chain U:

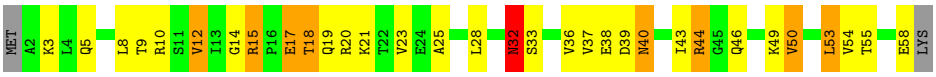


- Molecule 23: 50S ribosomal protein L29

Chain V:

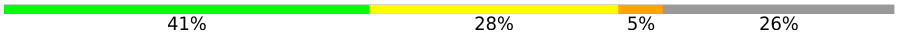
- Molecule 24: 50S ribosomal protein L30

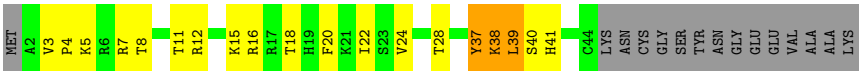
Chain W:



• Molecule 25: 50S ribosomal protein L32

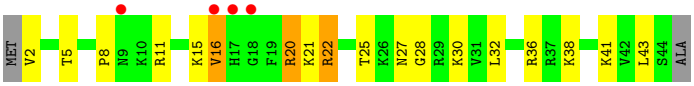
Chain Z:





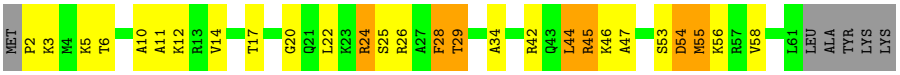
• Molecule 26: 50S ribosomal protein L34

Chain 2:



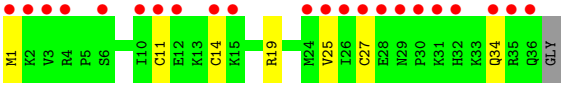
• Molecule 27: 50S ribosomal protein L35

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	282.11Å 282.11Å 875.34Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.93 – 3.55 49.93 – 3.55	Depositor EDS
% Data completeness (in resolution range)	95.4 (49.93-3.55) 95.4 (49.93-3.55)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.53 (at 3.57Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.187 , 0.227 0.189 , 0.227	Depositor DCC
R_{free} test set	11847 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	105.6	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.22 , 56.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	81462	wwPDB-VP
Average B, all atoms (Å^2)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.34% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, EPE, MN, EOH, MPD, SPD, 62B

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	A	0.26	0/1697	0.56	0/2332
2	X	0.96	108/64923 (0.2%)	1.63	1547/101215 (1.5%)
3	Y	0.90	10/2717 (0.4%)	1.73	90/4232 (2.1%)
4	B	0.68	0/1570	0.90	2/2117 (0.1%)
5	C	0.72	0/1343	0.98	1/1838 (0.1%)
6	D	0.33	0/855	0.56	0/1185
7	E	0.44	0/925	0.61	0/1279
8	G	0.78	0/1112	0.87	0/1507
9	H	0.62	0/891	0.80	0/1203
10	I	0.75	0/827	1.02	2/1121 (0.2%)
11	J	0.61	0/1023	0.80	0/1388
12	K	0.35	0/909	0.62	1/1217 (0.1%)
13	L	0.50	0/678	0.69	0/927
14	M	0.72	0/819	0.94	2/1107 (0.2%)
15	N	0.83	0/934	0.99	0/1241
16	O	0.84	1/761 (0.1%)	0.97	3/1022 (0.3%)
17	P	0.41	0/861	0.64	0/1160
18	Q	0.57	0/589	0.78	0/808
19	R	0.67	1/631 (0.2%)	0.85	0/863
20	S	0.60	0/1099	0.84	0/1509
21	T	0.59	0/565	0.79	0/751
22	U	0.37	0/247	0.57	0/344
23	V	0.50	0/487	0.64	0/654
24	W	0.73	0/439	0.93	0/593
25	Z	0.80	0/345	0.90	0/460
26	2	0.72	0/353	0.94	0/463
27	3	0.75	0/409	1.07	1/550 (0.2%)
28	4	0.41	0/180	0.66	0/249
All	All	0.89	120/88189 (0.1%)	1.50	1649/133335 (1.2%)

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
1	A	0	1
4	B	0	2
5	C	0	2
10	I	0	1
16	O	0	1
17	P	0	1
20	S	0	1
27	3	0	2
All	All	0	11

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	1186	A	N9-C4	-12.81	1.30	1.37
2	X	1289	A	N9-C4	-11.75	1.30	1.37
2	X	2845	G	N9-C4	-9.65	1.30	1.38
2	X	1065	A	N9-C4	-9.16	1.32	1.37
2	X	2740	A	N9-C4	-8.95	1.32	1.37

The worst 5 of 1649 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Y	93	C	N3-C2-O2	-20.18	107.77	121.90
2	X	2845	G	N3-C4-C5	18.48	137.84	128.60
3	Y	93	C	N1-C2-O2	16.73	128.94	118.90
2	X	1395	G	N1-C6-O6	-16.42	110.05	119.90
2	X	1289	A	C2-N3-C4	-16.32	102.44	110.60

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	77	LYS	Peptide
4	B	104	GLU	Peptide
4	B	57	LYS	Peptide
5	C	161	VAL	Peptide
5	C	27	GLU	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	A	1667	0	1292	51	0
2	X	57983	0	29161	923	0
3	Y	2430	0	1229	58	0
4	B	1547	0	1514	66	0
5	C	1324	0	1175	57	0
6	D	853	0	444	6	0
7	E	915	0	648	22	0
8	G	1090	0	1034	48	0
9	H	884	0	902	45	0
10	I	819	0	687	43	0
11	J	1001	0	971	37	0
12	K	906	0	930	36	0
13	L	673	0	538	19	0
14	M	807	0	803	32	0
15	N	922	0	973	61	0
16	O	751	0	743	22	0
17	P	853	0	900	30	0
18	Q	583	0	472	21	0
19	R	627	0	510	24	0
20	S	1087	0	934	26	0
21	T	559	0	569	24	0
22	U	242	0	141	4	0
23	V	486	0	469	10	0
24	W	437	0	467	26	0
25	Z	339	0	350	23	0
26	2	350	0	383	12	0
27	3	405	0	363	19	0
28	4	181	0	76	5	0
29	A	1	0	0	0	0
29	R	1	0	0	0	0
29	T	1	0	0	0	0
29	X	268	0	0	0	0
29	Y	2	0	0	0	0
29	Z	1	0	0	0	0
30	A	3	0	0	0	0
30	C	2	0	0	0	0
30	G	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	I	1	0	0	0	0
30	J	1	0	0	0	0
30	M	1	0	0	0	0
30	O	1	0	0	0	0
30	P	1	0	0	0	0
30	X	218	0	0	0	0
30	Y	10	0	0	0	0
31	X	35	0	0	1	0
32	J	8	0	14	1	0
32	Q	8	0	14	0	0
32	X	64	0	112	7	0
32	Z	8	0	14	0	0
33	X	70	0	133	9	0
33	Y	10	0	19	1	0
34	S	3	0	6	0	0
34	X	6	0	12	0	0
35	N	15	0	17	17	0
All	All	81462	0	49019	1574	0

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 12.

The worst 5 of 1574 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)
19:R:11:VAL:HA	19:R:67:ASN:HB2	1.48	0.96
2:X:956:A:H2'	11:J:11:ARG:HH11	1.30	0.96
2:X:83:G:H21	2:X:102:A:H2	1.15	0.93
4:B:124:GLY:HA2	4:B:174:GLY:HA3	1.53	0.91
3:Y:21:G:H1	3:Y:58:G:H1	1.08	0.91

There are no symmetry-related clashes.

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	
1	A	267/277 (96%)	222 (83%)	27 (10%)	18 (7%)	1	15
4	B	213/220 (97%)	187 (88%)	17 (8%)	9 (4%)	3	25
5	C	197/207 (95%)	155 (79%)	31 (16%)	11 (6%)	2	19
6	D	163/179 (91%)	131 (80%)	17 (10%)	15 (9%)	1	9
7	E	155/178 (87%)	120 (77%)	26 (17%)	9 (6%)	1	18
8	G	143/145 (99%)	131 (92%)	8 (6%)	4 (3%)	5	34
9	H	120/122 (98%)	102 (85%)	16 (13%)	2 (2%)	9	45
10	I	129/140 (92%)	91 (70%)	25 (19%)	13 (10%)	0	7
11	J	136/144 (94%)	110 (81%)	15 (11%)	11 (8%)	1	11
12	K	117/122 (96%)	101 (86%)	9 (8%)	7 (6%)	1	17
13	L	107/119 (90%)	86 (80%)	16 (15%)	5 (5%)	2	22
14	M	108/116 (93%)	85 (79%)	18 (17%)	5 (5%)	2	23
15	N	114/118 (97%)	108 (95%)	6 (5%)	0	100	100
16	O	100/102 (98%)	90 (90%)	5 (5%)	5 (5%)	2	21
17	P	110/117 (94%)	101 (92%)	8 (7%)	1 (1%)	17	57
18	Q	88/91 (97%)	74 (84%)	9 (10%)	5 (6%)	1	18
19	R	100/105 (95%)	71 (71%)	17 (17%)	12 (12%)	0	5
20	S	165/217 (76%)	121 (73%)	23 (14%)	21 (13%)	0	5
21	T	73/94 (78%)	63 (86%)	10 (14%)	0	100	100
22	U	40/62 (64%)	32 (80%)	6 (15%)	2 (5%)	2	21
23	V	63/69 (91%)	55 (87%)	5 (8%)	3 (5%)	2	22
24	W	55/59 (93%)	51 (93%)	3 (6%)	1 (2%)	8	43
25	Z	41/58 (71%)	36 (88%)	4 (10%)	1 (2%)	6	37
26	2	41/45 (91%)	39 (95%)	1 (2%)	1 (2%)	6	37
27	3	58/66 (88%)	42 (72%)	9 (16%)	7 (12%)	0	5
28	4	34/37 (92%)	26 (76%)	8 (24%)	0	100	100
All	All	2937/3209 (92%)	2430 (83%)	339 (12%)	168 (6%)	1	18

5 of 168 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	THR
1	A	35	LYS
1	A	36	PRO
1	A	51	VAL
1	A	78	VAL

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
1	A	112/224 (50%)	97 (87%)	15 (13%)	4 23
4	B	150/177 (85%)	121 (81%)	29 (19%)	1 8
5	C	106/169 (63%)	84 (79%)	22 (21%)	1 7
6	D	15/158 (10%)	13 (87%)	2 (13%)	4 23
7	E	51/156 (33%)	39 (76%)	12 (24%)	1 5
8	G	106/123 (86%)	87 (82%)	19 (18%)	2 11
9	H	91/100 (91%)	74 (81%)	17 (19%)	1 9
10	I	56/108 (52%)	39 (70%)	17 (30%)	0 3
11	J	90/119 (76%)	80 (89%)	10 (11%)	6 31
12	K	91/102 (89%)	77 (85%)	14 (15%)	2 18
13	L	40/95 (42%)	30 (75%)	10 (25%)	0 4
14	M	75/102 (74%)	53 (71%)	22 (29%)	0 3
15	N	91/98 (93%)	70 (77%)	21 (23%)	1 5
16	O	71/86 (83%)	63 (89%)	8 (11%)	6 30
17	P	89/94 (95%)	77 (86%)	12 (14%)	4 22
18	Q	41/82 (50%)	34 (83%)	7 (17%)	2 13
19	R	44/90 (49%)	26 (59%)	18 (41%)	0 1
20	S	88/190 (46%)	73 (83%)	15 (17%)	2 13
21	T	53/75 (71%)	40 (76%)	13 (24%)	0 4
22	U	8/52 (15%)	7 (88%)	1 (12%)	4 25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
23	V	47/62 (76%)	35 (74%)	12 (26%)	0 4
24	W	50/53 (94%)	38 (76%)	12 (24%)	0 4
25	Z	38/51 (74%)	32 (84%)	6 (16%)	2 17
26	2	35/40 (88%)	29 (83%)	6 (17%)	2 13
27	3	33/57 (58%)	27 (82%)	6 (18%)	1 10
28	4	2/35 (6%)	1 (50%)	1 (50%)	0 0
All	All	1673/2698 (62%)	1346 (80%)	327 (20%)	1 8

5 of 327 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	Q	49	LYS
23	V	23	GLU
19	R	4	LYS
20	S	41	VAL
24	W	32	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
14	M	14	GLN
16	O	63	ASN
17	P	40	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	X	2685/2923 (91%)	645 (24%)	36 (1%)
3	Y	113/114 (99%)	18 (15%)	0
All	All	2798/3037 (92%)	663 (23%)	36 (1%)

5 of 663 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	X	8	U
2	X	15	G
2	X	17	G
2	X	34	U

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Mol	Chain	Res	Type
2	X	38	A

5 of 36 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	X	1885	G
2	X	2611	U
2	X	1901	C
2	X	2378	G
2	X	890	G

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 538 ligands modelled in this entry, 514 are monoatomic - leaving 24 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	$\#\|Z\| > 2$
33	SPD	X	3498	-	9,9,9	0.38	0	8,8,8	0.61	0
33	SPD	X	3496	-	9,9,9	0.27	0	8,8,8	0.19	0
34	EOH	X	3500	-	2,2,2	0.62	0	1,1,1	0.50	0
32	MPD	X	3006	-	7,7,7	1.00	1 (14%)	9,10,10	0.56	0
33	SPD	Y	213	-	9,9,9	0.20	0	8,8,8	0.13	0
33	SPD	X	3493	-	9,9,9	0.33	0	8,8,8	0.53	0
35	EPE	N	201	-	15,15,15	1.14	1 (6%)	18,20,20	1.39	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
32	MPD	J	201	-	7,7,7	1.31	1 (14%)	9,10,10	0.69	0
32	MPD	X	3007	-	7,7,7	0.38	0	9,10,10	0.41	0
33	SPD	X	3497	-	9,9,9	0.12	0	8,8,8	0.34	0
31	62B	X	3003	-	37,38,38	1.03	2 (5%)	55,60,60	3.30	18 (32%)
32	MPD	X	3005	-	7,7,7	0.99	1 (14%)	9,10,10	0.66	0
32	MPD	X	3008	-	7,7,7	1.18	1 (14%)	9,10,10	0.68	0
33	SPD	X	3492	-	9,9,9	0.39	0	8,8,8	0.39	0
32	MPD	Z	101	-	7,7,7	0.62	0	9,10,10	0.22	0
32	MPD	X	3010	-	7,7,7	0.96	1 (14%)	9,10,10	0.42	0
32	MPD	Q	101	-	7,7,7	0.74	0	9,10,10	0.26	0
33	SPD	X	3495	-	9,9,9	0.24	0	8,8,8	0.36	0
34	EOH	X	3499	-	2,2,2	0.62	0	1,1,1	0.48	0
34	EOH	S	301	-	2,2,2	0.71	0	1,1,1	0.29	0
32	MPD	X	3004	-	7,7,7	1.16	1 (14%)	9,10,10	0.71	0
33	SPD	X	3494	-	9,9,9	0.21	0	8,8,8	0.31	0
32	MPD	X	3011	-	7,7,7	1.27	1 (14%)	9,10,10	0.46	0
32	MPD	X	3009	-	7,7,7	0.62	0	9,10,10	0.30	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
33	SPD	X	3498	-	-	3/7/7/7	-
33	SPD	X	3496	-	-	1/7/7/7	-
32	MPD	X	3006	-	-	1/5/5/5	-
33	SPD	Y	213	-	-	2/7/7/7	-
33	SPD	X	3493	-	-	1/7/7/7	-
35	EPE	N	201	-	-	5/9/19/19	0/1/1/1
32	MPD	J	201	-	-	1/5/5/5	-
32	MPD	X	3007	-	-	0/5/5/5	-
33	SPD	X	3497	-	-	4/7/7/7	-
31	62B	X	3003	-	-	1/12/86/86	0/4/4/4
32	MPD	X	3005	-	-	2/5/5/5	-
32	MPD	X	3008	-	-	3/5/5/5	-
33	SPD	X	3492	-	-	4/7/7/7	-
32	MPD	Z	101	-	-	1/5/5/5	-
32	MPD	X	3010	-	-	1/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	MPD	Q	101	-	-	1/5/5/5	-
33	SPD	X	3495	-	-	5/7/7/7	-
32	MPD	X	3004	-	-	4/5/5/5	-
33	SPD	X	3494	-	-	3/7/7/7	-
32	MPD	X	3011	-	-	3/5/5/5	-
32	MPD	X	3009	-	-	2/5/5/5	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	X	3003	62B	C10-C11	4.35	1.60	1.56
35	N	201	EPE	C10-S	-3.77	1.72	1.77
31	X	3003	62B	C13-C12	-3.24	1.49	1.55
32	J	201	MPD	C3-C2	2.99	1.61	1.53
32	X	3011	MPD	C3-C2	2.81	1.61	1.53

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	X	3003	62B	C18-C12-C11	12.98	115.64	108.06
31	X	3003	62B	C15-C5-C14	-8.58	100.50	108.95
31	X	3003	62B	C6-C5-C14	7.47	117.16	112.10
31	X	3003	62B	C24-C25-C26	-7.23	103.25	111.53
31	X	3003	62B	C13-C12-C19	-6.16	98.31	111.04

There are no chirality outliers.

5 of 48 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	X	3004	MPD	O2-C2-C3-C4
32	X	3004	MPD	C2-C3-C4-O4
35	N	201	EPE	N4-C7-C8-O8
33	X	3495	SPD	N6-C7-C8-C9
33	X	3498	SPD	C8-C7-N6-C5

There are no ring outliers.

14 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	X	3498	SPD	1	0

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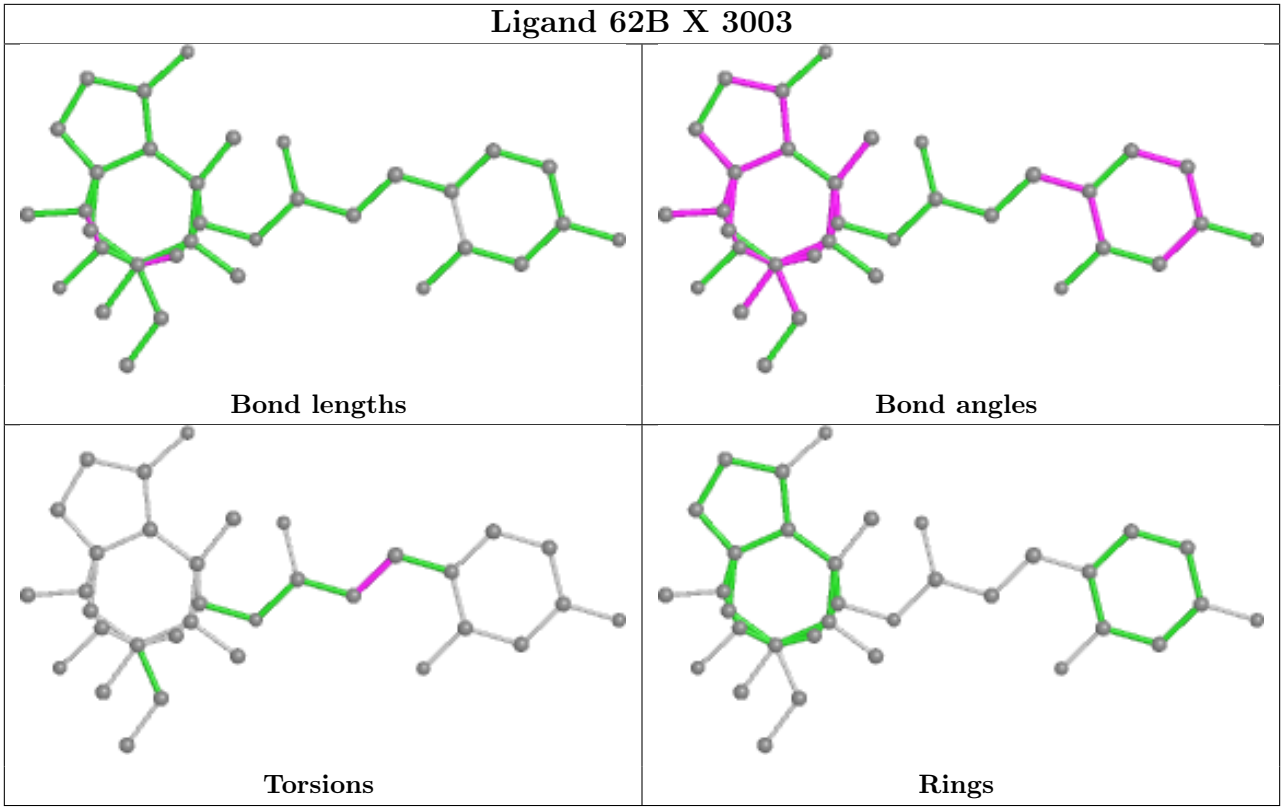
Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	X	3006	MPD	2	0
33	Y	213	SPD	1	0
33	X	3493	SPD	2	0
35	N	201	EPE	17	0
32	J	201	MPD	1	0
33	X	3497	SPD	3	0
31	X	3003	62B	1	0
32	X	3005	MPD	1	0
32	X	3008	MPD	1	0
32	X	3010	MPD	1	0
33	X	3495	SPD	2	0
32	X	3004	MPD	2	0
33	X	3494	SPD	1	0

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 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.



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

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	A	269/277 (97%)	-0.31	4 (1%)	73	59	92, 138, 160, 172	0
2	X	2705/2923 (92%)	-0.49	17 (0%)	89	80	53, 101, 188, 280	0
3	Y	114/114 (100%)	-0.63	0	100	100	76, 125, 175, 180	0
4	B	215/220 (97%)	-0.31	1 (0%)	91	83	62, 81, 99, 116	0
5	C	199/207 (96%)	-0.43	1 (0%)	91	83	64, 96, 113, 138	0
6	D	165/179 (92%)	0.02	11 (6%)	17	11	166, 193, 231, 239	0
7	E	157/178 (88%)	-0.26	6 (3%)	40	27	133, 172, 206, 212	0
8	G	145/145 (100%)	-0.20	1 (0%)	87	78	64, 79, 91, 96	0
9	H	122/122 (100%)	-0.37	0	100	100	84, 102, 123, 128	0
10	I	131/140 (93%)	-0.02	5 (3%)	40	27	58, 116, 136, 142	0
11	J	138/144 (95%)	0.24	4 (2%)	51	35	77, 103, 135, 152	0
12	K	119/122 (97%)	-0.54	0	100	100	67, 84, 108, 141	0
13	L	109/119 (91%)	-0.83	0	100	100	121, 130, 157, 189	0
14	M	110/116 (94%)	-0.39	2 (1%)	68	52	85, 99, 132, 156	0
15	N	116/118 (98%)	-0.43	0	100	100	54, 70, 90, 96	0
16	O	102/102 (100%)	-0.56	0	100	100	54, 88, 103, 109	0
17	P	112/117 (95%)	-0.01	1 (0%)	84	72	64, 75, 114, 139	0
18	Q	90/91 (98%)	-0.19	0	100	100	98, 122, 138, 170	0
19	R	102/105 (97%)	0.30	6 (5%)	22	13	98, 121, 189, 206	0
20	S	167/217 (76%)	-0.27	1 (0%)	89	80	87, 109, 199, 218	0
21	T	75/94 (79%)	-0.00	1 (1%)	77	63	85, 97, 115, 129	0
22	U	42/62 (67%)	2.37	24 (57%)	0	0	160, 172, 203, 213	0
23	V	65/69 (94%)	-0.07	0	100	100	134, 145, 159, 163	0
24	W	57/59 (96%)	0.21	0	100	100	63, 77, 99, 101	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
25	Z	43/58 (74%)	-0.26	0	100	100	54, 76, 131, 136	0
26	2	43/45 (95%)	0.41	4 (9%)	8	5	83, 92, 102, 105	0
27	3	60/66 (90%)	-0.24	0	100	100	80, 89, 105, 109	0
28	4	36/37 (97%)	2.40	22 (61%)	0	0	159, 164, 174, 178	0
All	All	5808/6246 (92%)	-0.32	111 (1%)	66	50	53, 103, 190, 280	0

The worst 5 of 111 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	U	16	ASN	5.7
22	U	30	ASN	5.4
28	4	32	HIS	5.2
22	U	27	ARG	5.1
28	4	30	PRO	5.0

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
30	MG	Y	210	1/1	0.17	1.31	105,105,105,105	0
30	MG	X	3250	1/1	0.21	1.64	89,89,89,89	0
29	MN	X	3466	1/1	0.37	0.38	155,155,155,155	0
30	MG	X	3306	1/1	0.43	0.43	95,95,95,95	0
29	MN	X	3209	1/1	0.43	0.19	150,150,150,150	0
30	MG	X	3340	1/1	0.45	0.64	84,84,84,84	0
30	MG	X	3351	1/1	0.46	0.63	116,116,116,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	MG	X	3449	1/1	0.47	0.42	86,86,86,86	0
30	MG	X	3417	1/1	0.47	0.93	82,82,82,82	0
29	MN	X	3437	1/1	0.49	0.13	153,153,153,153	0
30	MG	X	3474	1/1	0.53	0.23	106,106,106,106	0
29	MN	X	3460	1/1	0.53	0.36	182,182,182,182	0
30	MG	X	3362	1/1	0.54	0.36	114,114,114,114	0
30	MG	X	3337	1/1	0.55	0.47	89,89,89,89	0
30	MG	Y	203	1/1	0.55	0.60	96,96,96,96	0
30	MG	X	3349	1/1	0.55	1.47	127,127,127,127	0
30	MG	X	3180	1/1	0.56	1.15	78,78,78,78	0
30	MG	X	3488	1/1	0.57	0.67	100,100,100,100	0
30	MG	X	3310	1/1	0.57	0.22	129,129,129,129	0
30	MG	X	3487	1/1	0.57	0.53	109,109,109,109	0
30	MG	X	3391	1/1	0.58	1.00	107,107,107,107	0
30	MG	X	3327	1/1	0.58	1.10	126,126,126,126	0
30	MG	X	3400	1/1	0.60	0.63	90,90,90,90	0
30	MG	X	3433	1/1	0.60	0.34	124,124,124,124	0
30	MG	X	3341	1/1	0.61	0.64	96,96,96,96	0
29	MN	X	3211	1/1	0.61	0.35	144,144,144,144	0
30	MG	A	303	1/1	0.62	0.31	94,94,94,94	0
29	MN	X	3324	1/1	0.62	0.16	164,164,164,164	0
30	MG	X	3308	1/1	0.63	0.44	77,77,77,77	0
30	MG	X	3335	1/1	0.63	0.70	61,61,61,61	0
30	MG	Y	212	1/1	0.64	0.63	95,95,95,95	0
29	MN	X	3471	1/1	0.66	1.22	130,130,130,130	0
29	MN	X	3446	1/1	0.66	0.45	142,142,142,142	0
30	MG	X	3087	1/1	0.66	0.66	55,55,55,55	0
30	MG	X	3344	1/1	0.66	0.85	91,91,91,91	0
29	MN	X	3202	1/1	0.66	0.22	173,173,173,173	0
29	MN	X	3263	1/1	0.66	0.35	166,166,166,166	0
29	MN	X	3421	1/1	0.67	0.45	111,111,111,111	0
30	MG	X	3393	1/1	0.67	1.22	104,104,104,104	0
30	MG	X	3248	1/1	0.68	0.55	69,69,69,69	0
30	MG	X	3294	1/1	0.68	0.45	108,108,108,108	0
30	MG	X	3445	1/1	0.69	1.41	104,104,104,104	0
30	MG	X	3386	1/1	0.69	0.40	88,88,88,88	0
30	MG	X	3253	1/1	0.69	1.55	112,112,112,112	0
30	MG	X	3435	1/1	0.69	0.28	153,153,153,153	0
33	SPD	X	3498	10/10	0.69	0.41	93,93,93,93	0
30	MG	X	3357	1/1	0.70	0.29	95,95,95,95	0
29	MN	X	3181	1/1	0.70	0.12	142,142,142,142	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
29	MN	X	3183	1/1	0.71	0.14	125,125,125,125	0
29	MN	X	3114	1/1	0.71	0.56	122,122,122,122	0
30	MG	X	3358	1/1	0.71	1.38	88,88,88,88	0
29	MN	X	3203	1/1	0.71	0.19	145,145,145,145	0
30	MG	X	3370	1/1	0.71	1.18	113,113,113,113	0
30	MG	X	3475	1/1	0.71	0.85	93,93,93,93	0
30	MG	X	3395	1/1	0.72	0.37	79,79,79,79	0
30	MG	X	3196	1/1	0.72	0.52	89,89,89,89	0
30	MG	G	202	1/1	0.72	0.37	77,77,77,77	0
30	MG	X	3222	1/1	0.72	0.21	80,80,80,80	0
29	MN	X	3425	1/1	0.73	0.30	101,101,101,101	0
29	MN	X	3225	1/1	0.73	0.53	157,157,157,157	0
30	MG	X	3428	1/1	0.73	0.12	105,105,105,105	0
30	MG	X	3254	1/1	0.73	0.77	66,66,66,66	0
30	MG	X	3293	1/1	0.73	0.47	117,117,117,117	0
30	MG	X	3236	1/1	0.73	0.71	88,88,88,88	0
29	MN	X	3210	1/1	0.73	0.22	201,201,201,201	0
30	MG	X	3398	1/1	0.73	0.59	99,99,99,99	0
30	MG	X	3361	1/1	0.74	0.37	86,86,86,86	0
30	MG	X	3255	1/1	0.74	0.62	94,94,94,94	0
30	MG	P	201	1/1	0.74	0.65	63,63,63,63	0
30	MG	X	3230	1/1	0.74	0.54	80,80,80,80	0
34	EOH	S	301	3/3	0.74	0.35	90,90,90,90	0
30	MG	X	3252	1/1	0.75	1.35	114,114,114,114	0
29	MN	X	3072	1/1	0.75	0.21	123,123,123,123	0
29	MN	X	3155	1/1	0.75	0.40	110,110,110,110	0
30	MG	X	3265	1/1	0.76	0.64	96,96,96,96	0
30	MG	X	3348	1/1	0.76	0.62	72,72,72,72	0
30	MG	X	3266	1/1	0.76	0.34	90,90,90,90	0
29	MN	X	3458	1/1	0.76	0.54	127,127,127,127	0
30	MG	X	3441	1/1	0.76	0.57	96,96,96,96	0
30	MG	G	201	1/1	0.76	0.57	89,89,89,89	0
30	MG	X	3352	1/1	0.76	0.52	94,94,94,94	0
30	MG	X	3244	1/1	0.76	0.51	109,109,109,109	0
29	MN	X	3166	1/1	0.76	0.21	92,92,92,92	0
29	MN	X	3478	1/1	0.76	0.20	132,132,132,132	0
29	MN	X	3112	1/1	0.77	0.25	124,124,124,124	0
30	MG	X	3339	1/1	0.77	1.67	108,108,108,108	0
29	MN	X	3175	1/1	0.77	0.28	122,122,122,122	0
30	MG	A	302	1/1	0.78	0.57	92,92,92,92	0
30	MG	X	3346	1/1	0.78	0.47	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	MPD	J	201	8/8	0.78	0.30	125,125,125,125	0
30	MG	X	3336	1/1	0.78	0.91	99,99,99,99	0
33	SPD	Y	213	10/10	0.78	0.38	101,101,101,101	0
30	MG	X	3342	1/1	0.78	0.52	80,80,80,80	0
30	MG	X	3332	1/1	0.79	0.44	81,81,81,81	0
30	MG	X	3130	1/1	0.79	0.36	72,72,72,72	0
29	MN	X	3447	1/1	0.79	0.24	128,128,128,128	0
32	MPD	X	3004	8/8	0.79	0.30	135,135,135,135	0
29	MN	X	3186	1/1	0.79	0.45	143,143,143,143	0
30	MG	X	3286	1/1	0.79	0.47	77,77,77,77	0
29	MN	X	3379	1/1	0.79	0.19	158,158,158,158	0
30	MG	X	3365	1/1	0.79	0.69	76,76,76,76	0
29	MN	Z	102	1/1	0.80	0.36	112,112,112,112	0
30	MG	X	3394	1/1	0.80	0.19	98,98,98,98	0
29	MN	X	3454	1/1	0.80	0.49	126,126,126,126	0
30	MG	X	3382	1/1	0.80	0.66	126,126,126,126	0
29	MN	X	3158	1/1	0.80	0.30	117,117,117,117	0
30	MG	X	3413	1/1	0.80	0.56	90,90,90,90	0
29	MN	X	3231	1/1	0.80	0.26	161,161,161,161	0
30	MG	X	3423	1/1	0.81	0.32	79,79,79,79	0
30	MG	Y	207	1/1	0.81	0.27	78,78,78,78	0
30	MG	X	3385	1/1	0.81	1.06	88,88,88,88	0
30	MG	X	3229	1/1	0.81	0.20	98,98,98,98	0
29	MN	X	3468	1/1	0.81	0.25	104,104,104,104	0
29	MN	X	3469	1/1	0.81	0.17	140,140,140,140	0
29	MN	X	3323	1/1	0.81	0.26	141,141,141,141	0
29	MN	X	3185	1/1	0.81	0.16	101,101,101,101	0
29	MN	X	3146	1/1	0.81	0.20	122,122,122,122	0
33	SPD	X	3496	10/10	0.81	0.48	102,102,102,102	0
29	MN	X	3314	1/1	0.81	0.30	147,147,147,147	0
30	MG	X	3375	1/1	0.81	0.24	76,76,76,76	0
30	MG	X	3228	1/1	0.81	0.30	150,150,150,150	0
30	MG	X	3260	1/1	0.82	0.14	123,123,123,123	0
30	MG	X	3378	1/1	0.82	0.59	83,83,83,83	0
29	MN	X	3456	1/1	0.82	0.24	113,113,113,113	0
30	MG	X	3354	1/1	0.82	0.71	75,75,75,75	0
29	MN	X	3154	1/1	0.82	0.35	124,124,124,124	0
30	MG	X	3212	1/1	0.82	0.97	78,78,78,78	0
30	MG	X	3288	1/1	0.82	0.32	81,81,81,81	0
29	MN	X	3479	1/1	0.82	0.24	171,171,171,171	0
30	MG	X	3363	1/1	0.82	0.36	82,82,82,82	0
29	MN	X	3162	1/1	0.82	0.24	118,118,118,118	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	MG	X	3305	1/1	0.82	0.43	123,123,123,123	0
30	MG	X	3406	1/1	0.82	0.29	71,71,71,71	0
30	MG	X	3408	1/1	0.82	1.48	97,97,97,97	0
30	MG	X	3429	1/1	0.83	0.23	102,102,102,102	0
30	MG	X	3477	1/1	0.83	0.32	80,80,80,80	0
30	MG	X	3123	1/1	0.83	0.49	69,69,69,69	0
30	MG	X	3307	1/1	0.83	0.52	71,71,71,71	0
29	MN	X	3133	1/1	0.83	0.28	133,133,133,133	0
32	MPD	Q	101	8/8	0.83	0.20	137,137,137,137	0
30	MG	X	3167	1/1	0.83	0.34	62,62,62,62	0
30	MG	X	3213	1/1	0.83	1.50	86,86,86,86	0
30	MG	X	3356	1/1	0.83	0.13	83,83,83,83	0
30	MG	C	302	1/1	0.83	0.29	78,78,78,78	0
29	MN	X	3208	1/1	0.84	0.29	141,141,141,141	0
29	MN	X	3168	1/1	0.84	0.29	115,115,115,115	0
30	MG	X	3345	1/1	0.84	0.30	65,65,65,65	0
29	MN	X	3360	1/1	0.84	0.12	146,146,146,146	0
30	MG	X	3387	1/1	0.84	0.34	175,175,175,175	0
30	MG	X	3246	1/1	0.84	0.90	72,72,72,72	0
29	MN	X	3463	1/1	0.84	0.17	134,134,134,134	0
29	MN	X	3174	1/1	0.84	0.18	121,121,121,121	0
30	MG	X	3489	1/1	0.84	0.70	62,62,62,62	0
30	MG	X	3283	1/1	0.84	0.22	129,129,129,129	0
29	MN	X	3139	1/1	0.84	0.45	117,117,117,117	0
30	MG	X	3440	1/1	0.84	0.42	79,79,79,79	0
29	MN	X	3316	1/1	0.85	0.10	173,173,173,173	0
30	MG	X	3002	1/1	0.85	1.02	100,100,100,100	0
30	MG	X	3280	1/1	0.85	0.33	159,159,159,159	0
30	MG	X	3300	1/1	0.85	0.25	94,94,94,94	0
32	MPD	X	3008	8/8	0.85	0.26	94,94,94,94	0
30	MG	X	3371	1/1	0.85	0.49	88,88,88,88	0
30	MG	Y	205	1/1	0.85	0.82	94,94,94,94	0
33	SPD	X	3492	10/10	0.85	0.27	105,105,105,105	0
30	MG	X	3372	1/1	0.85	0.50	78,78,78,78	0
33	SPD	X	3497	10/10	0.85	0.18	96,96,96,96	0
30	MG	X	3419	1/1	0.85	0.70	107,107,107,107	0
29	MN	X	3319	1/1	0.85	0.10	158,158,158,158	0
29	MN	X	3150	1/1	0.85	0.18	110,110,110,110	0
30	MG	X	3224	1/1	0.86	0.78	66,66,66,66	0
30	MG	X	3242	1/1	0.86	0.69	65,65,65,65	0
32	MPD	Z	101	8/8	0.86	0.21	145,145,145,145	0
30	MG	X	3329	1/1	0.86	0.52	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
33	SPD	X	3494	10/10	0.86	0.27	87,87,87,87	0
29	MN	X	3178	1/1	0.86	0.11	126,126,126,126	0
30	MG	X	3444	1/1	0.86	0.40	100,100,100,100	0
29	MN	X	3262	1/1	0.86	0.12	143,143,143,143	0
29	MN	X	3148	1/1	0.86	0.25	144,144,144,144	0
30	MG	X	3233	1/1	0.86	0.34	68,68,68,68	0
30	MG	X	3129	1/1	0.87	0.60	79,79,79,79	0
29	MN	Y	208	1/1	0.87	0.19	164,164,164,164	0
29	MN	X	3380	1/1	0.87	0.26	151,151,151,151	0
29	MN	X	3194	1/1	0.87	0.21	138,138,138,138	0
29	MN	X	3422	1/1	0.87	0.23	154,154,154,154	0
30	MG	X	3328	1/1	0.87	0.53	103,103,103,103	0
29	MN	X	3058	1/1	0.87	0.39	101,101,101,101	0
30	MG	X	3347	1/1	0.87	1.25	108,108,108,108	0
30	MG	X	3411	1/1	0.87	0.42	82,82,82,82	0
30	MG	X	3241	1/1	0.87	1.25	78,78,78,78	0
30	MG	X	3334	1/1	0.87	0.70	89,89,89,89	0
30	MG	X	3350	1/1	0.87	0.39	100,100,100,100	0
33	SPD	X	3495	10/10	0.87	0.24	83,83,83,83	0
30	MG	X	3504	1/1	0.87	0.57	74,74,74,74	0
30	MG	X	3295	1/1	0.87	0.45	100,100,100,100	0
29	MN	X	3376	1/1	0.87	0.10	119,119,119,119	0
29	MN	X	3116	1/1	0.87	0.42	111,111,111,111	0
30	MG	X	3338	1/1	0.87	0.34	82,82,82,82	0
29	MN	X	3176	1/1	0.88	0.31	128,128,128,128	0
30	MG	X	3287	1/1	0.88	1.56	102,102,102,102	0
30	MG	J	202	1/1	0.88	0.18	92,92,92,92	0
29	MN	X	3320	1/1	0.88	0.31	107,107,107,107	0
30	MG	X	3290	1/1	0.88	0.59	98,98,98,98	0
30	MG	X	3412	1/1	0.88	0.53	106,106,106,106	0
32	MPD	X	3010	8/8	0.88	0.22	113,113,113,113	0
30	MG	X	3144	1/1	0.88	0.32	71,71,71,71	0
30	MG	X	3226	1/1	0.88	0.82	102,102,102,102	0
30	MG	X	3359	1/1	0.88	0.51	91,91,91,91	0
30	MG	X	3420	1/1	0.88	0.47	75,75,75,75	0
29	MN	X	3113	1/1	0.88	0.23	96,96,96,96	0
29	MN	X	3461	1/1	0.88	0.26	149,149,149,149	0
29	MN	X	3151	1/1	0.88	0.25	97,97,97,97	0
30	MG	X	3282	1/1	0.88	0.25	85,85,85,85	0
30	MG	X	3368	1/1	0.88	0.54	87,87,87,87	0
30	MG	X	3397	1/1	0.88	0.21	78,78,78,78	0
29	MN	X	3182	1/1	0.88	0.13	133,133,133,133	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	MG	X	3298	1/1	0.89	0.40	95,95,95,95	0
29	MN	X	3060	1/1	0.89	0.23	90,90,90,90	0
29	MN	X	3025	1/1	0.89	0.31	128,128,128,128	0
30	MG	X	3484	1/1	0.89	0.17	77,77,77,77	0
30	MG	X	3238	1/1	0.89	0.86	85,85,85,85	0
30	MG	X	3424	1/1	0.89	1.44	89,89,89,89	0
29	MN	X	3153	1/1	0.89	0.09	123,123,123,123	0
29	MN	X	3019	1/1	0.89	0.32	109,109,109,109	0
29	MN	X	3124	1/1	0.89	0.13	147,147,147,147	0
33	SPD	X	3493	10/10	0.89	0.27	83,83,83,83	0
30	MG	X	3291	1/1	0.89	0.47	86,86,86,86	0
30	MG	X	3355	1/1	0.89	0.19	91,91,91,91	0
30	MG	X	3205	1/1	0.89	0.15	98,98,98,98	0
30	MG	X	3343	1/1	0.89	0.63	73,73,73,73	0
29	MN	X	3326	1/1	0.89	0.21	145,145,145,145	0
30	MG	X	3249	1/1	0.89	0.98	109,109,109,109	0
30	MG	X	3473	1/1	0.89	0.19	82,82,82,82	0
29	MN	X	3084	1/1	0.90	0.14	123,123,123,123	0
30	MG	X	3138	1/1	0.90	0.53	72,72,72,72	0
29	MN	X	3198	1/1	0.90	0.18	125,125,125,125	0
30	MG	X	3381	1/1	0.90	0.71	97,97,97,97	0
30	MG	X	3416	1/1	0.90	0.27	90,90,90,90	0
30	MG	X	3232	1/1	0.90	1.01	74,74,74,74	0
29	MN	R	201	1/1	0.90	0.28	123,123,123,123	0
30	MG	X	3486	1/1	0.90	0.60	90,90,90,90	0
29	MN	X	3147	1/1	0.90	0.11	119,119,119,119	0
29	MN	X	3465	1/1	0.90	0.24	117,117,117,117	0
29	MN	X	3117	1/1	0.90	0.26	107,107,107,107	0
30	MG	X	3207	1/1	0.90	0.28	66,66,66,66	0
30	MG	A	304	1/1	0.90	0.49	105,105,105,105	0
29	MN	X	3119	1/1	0.90	0.20	140,140,140,140	0
30	MG	X	3214	1/1	0.90	0.77	86,86,86,86	0
29	MN	X	3034	1/1	0.90	0.26	77,77,77,77	0
30	MG	Y	211	1/1	0.90	0.42	115,115,115,115	0
29	MN	X	3027	1/1	0.90	0.36	68,68,68,68	0
34	EOH	X	3500	3/3	0.90	0.34	99,99,99,99	0
29	MN	X	3073	1/1	0.90	0.36	95,95,95,95	0
30	MG	X	3443	1/1	0.91	0.24	118,118,118,118	0
29	MN	X	3453	1/1	0.91	0.33	126,126,126,126	0
29	MN	X	3184	1/1	0.91	0.13	128,128,128,128	0
30	MG	X	3448	1/1	0.91	0.65	72,72,72,72	0
30	MG	X	3268	1/1	0.91	0.36	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	MG	X	3304	1/1	0.91	0.46	117,117,117,117	0
30	MG	M	201	1/1	0.91	0.42	68,68,68,68	0
30	MG	O	201	1/1	0.91	0.27	51,51,51,51	0
29	MN	X	3045	1/1	0.91	0.27	96,96,96,96	0
29	MN	X	3110	1/1	0.91	0.19	117,117,117,117	0
32	MPD	X	3006	8/8	0.91	0.22	82,82,82,82	0
29	MN	X	3480	1/1	0.91	0.57	175,175,175,175	0
30	MG	X	3481	1/1	0.91	0.23	82,82,82,82	0
30	MG	X	3285	1/1	0.91	0.21	75,75,75,75	0
30	MG	X	3485	1/1	0.91	0.23	102,102,102,102	0
29	MN	A	301	1/1	0.91	0.39	138,138,138,138	0
29	MN	X	3315	1/1	0.91	0.18	104,104,104,104	0
29	MN	X	3462	1/1	0.91	0.28	152,152,152,152	0
29	MN	X	3439	1/1	0.91	0.28	94,94,94,94	0
30	MG	X	3490	1/1	0.91	0.30	100,100,100,100	0
30	MG	X	3396	1/1	0.91	0.60	108,108,108,108	0
29	MN	X	3059	1/1	0.91	0.24	111,111,111,111	0
29	MN	X	3159	1/1	0.91	0.17	118,118,118,118	0
30	MG	Y	206	1/1	0.91	0.86	104,104,104,104	0
30	MG	X	3399	1/1	0.91	0.47	79,79,79,79	0
29	MN	X	3452	1/1	0.91	0.08	120,120,120,120	0
35	EPE	N	201	15/15	0.91	0.20	73,73,73,73	0
30	MG	X	3165	1/1	0.92	0.79	84,84,84,84	0
29	MN	T	101	1/1	0.92	0.18	121,121,121,121	0
29	MN	X	3077	1/1	0.92	0.32	100,100,100,100	0
29	MN	X	3111	1/1	0.92	0.32	130,130,130,130	0
30	MG	X	3483	1/1	0.92	0.29	91,91,91,91	0
30	MG	X	3333	1/1	0.92	0.77	97,97,97,97	0
30	MG	X	3259	1/1	0.92	0.49	122,122,122,122	0
32	MPD	X	3007	8/8	0.92	0.36	132,132,132,132	0
30	MG	X	3383	1/1	0.92	0.46	75,75,75,75	0
29	MN	X	3177	1/1	0.92	0.16	125,125,125,125	0
32	MPD	X	3011	8/8	0.92	0.30	75,75,75,75	0
29	MN	X	3044	1/1	0.92	0.37	116,116,116,116	0
29	MN	X	3405	1/1	0.92	0.17	103,103,103,103	0
29	MN	X	3455	1/1	0.92	0.43	116,116,116,116	0
30	MG	X	3302	1/1	0.92	0.16	100,100,100,100	0
30	MG	X	3303	1/1	0.92	0.72	101,101,101,101	0
30	MG	Y	204	1/1	0.92	0.37	78,78,78,78	0
30	MG	X	3272	1/1	0.92	0.46	104,104,104,104	0
29	MN	X	3101	1/1	0.92	0.48	131,131,131,131	0
29	MN	X	3322	1/1	0.92	0.15	137,137,137,137	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
29	MN	X	3199	1/1	0.92	0.20	143,143,143,143	0
30	MG	X	3367	1/1	0.92	0.39	83,83,83,83	0
29	MN	X	3173	1/1	0.92	0.25	129,129,129,129	0
30	MG	X	3369	1/1	0.92	0.74	70,70,70,70	0
29	MN	X	3109	1/1	0.92	0.14	92,92,92,92	0
29	MN	X	3024	1/1	0.93	0.18	120,120,120,120	0
29	MN	X	3470	1/1	0.93	0.18	148,148,148,148	0
29	MN	X	3163	1/1	0.93	0.13	124,124,124,124	0
29	MN	X	3190	1/1	0.93	0.20	124,124,124,124	0
29	MN	X	3317	1/1	0.93	0.14	137,137,137,137	0
30	MG	X	3388	1/1	0.93	0.85	85,85,85,85	0
30	MG	X	3137	1/1	0.93	1.13	63,63,63,63	0
32	MPD	X	3009	8/8	0.93	0.39	129,129,129,129	0
29	MN	X	3104	1/1	0.93	0.14	94,94,94,94	0
29	MN	X	3157	1/1	0.93	0.24	108,108,108,108	0
30	MG	X	3434	1/1	0.93	0.21	64,64,64,64	0
29	MN	X	3321	1/1	0.93	0.07	159,159,159,159	0
29	MN	X	3122	1/1	0.93	0.23	99,99,99,99	0
30	MG	X	3258	1/1	0.93	0.26	80,80,80,80	0
30	MG	X	3292	1/1	0.93	0.36	89,89,89,89	0
29	MN	X	3243	1/1	0.93	0.18	114,114,114,114	0
29	MN	X	3071	1/1	0.93	0.21	98,98,98,98	0
29	MN	X	3161	1/1	0.93	0.23	93,93,93,93	0
30	MG	X	3373	1/1	0.93	0.33	97,97,97,97	0
30	MG	X	3297	1/1	0.93	0.19	81,81,81,81	0
30	MG	X	3353	1/1	0.93	0.17	79,79,79,79	0
34	EOH	X	3499	3/3	0.93	0.40	80,80,80,80	0
29	MN	X	3311	1/1	0.93	0.16	124,124,124,124	0
30	MG	I	201	1/1	0.93	0.57	80,80,80,80	0
30	MG	X	3415	1/1	0.93	0.24	81,81,81,81	0
30	MG	X	3274	1/1	0.94	0.34	99,99,99,99	0
29	MN	X	3037	1/1	0.94	0.26	90,90,90,90	0
29	MN	X	3149	1/1	0.94	0.26	109,109,109,109	0
30	MG	X	3390	1/1	0.94	0.56	63,63,63,63	0
30	MG	X	3427	1/1	0.94	0.15	59,59,59,59	0
29	MN	X	3082	1/1	0.94	0.20	112,112,112,112	0
29	MN	X	3125	1/1	0.94	0.13	123,123,123,123	0
29	MN	X	3318	1/1	0.94	0.08	128,128,128,128	0
30	MG	X	3501	1/1	0.94	0.83	64,64,64,64	0
30	MG	X	3366	1/1	0.94	0.66	99,99,99,99	0
30	MG	X	3142	1/1	0.94	0.51	72,72,72,72	0
30	MG	X	3309	1/1	0.94	0.34	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
29	MN	X	3193	1/1	0.94	0.09	110,110,110,110	0
29	MN	X	3115	1/1	0.94	0.32	116,116,116,116	0
29	MN	X	3237	1/1	0.94	0.07	167,167,167,167	0
29	MN	X	3179	1/1	0.94	0.12	106,106,106,106	0
29	MN	X	3041	1/1	0.94	0.18	77,77,77,77	0
29	MN	X	3094	1/1	0.94	0.14	124,124,124,124	0
30	MG	X	3450	1/1	0.94	0.75	132,132,132,132	0
30	MG	X	3239	1/1	0.94	0.39	91,91,91,91	0
30	MG	X	3240	1/1	0.94	0.67	78,78,78,78	0
29	MN	X	3264	1/1	0.94	0.12	117,117,117,117	0
29	MN	X	3047	1/1	0.94	0.26	70,70,70,70	0
30	MG	X	3301	1/1	0.94	0.19	72,72,72,72	0
29	MN	X	3192	1/1	0.95	0.09	138,138,138,138	0
29	MN	X	3036	1/1	0.95	0.30	86,86,86,86	0
29	MN	X	3464	1/1	0.95	0.56	149,149,149,149	0
29	MN	X	3017	1/1	0.95	0.08	92,92,92,92	0
30	MG	X	3247	1/1	0.95	0.52	85,85,85,85	0
30	MG	X	3432	1/1	0.95	0.24	71,71,71,71	0
29	MN	X	3404	1/1	0.95	0.15	131,131,131,131	0
29	MN	X	3197	1/1	0.95	0.26	138,138,138,138	0
30	MG	X	3384	1/1	0.95	0.26	102,102,102,102	0
30	MG	X	3438	1/1	0.95	0.20	84,84,84,84	0
29	MN	X	3407	1/1	0.95	0.20	83,83,83,83	0
30	MG	X	3299	1/1	0.95	0.22	149,149,149,149	0
29	MN	X	3418	1/1	0.95	0.13	124,124,124,124	0
30	MG	X	3204	1/1	0.95	0.14	100,100,100,100	0
29	MN	X	3090	1/1	0.95	0.26	97,97,97,97	0
31	62B	X	3003	35/35	0.95	0.29	65,65,65,65	0
29	MN	X	3128	1/1	0.95	0.24	93,93,93,93	0
32	MPD	X	3005	8/8	0.95	0.23	78,78,78,78	0
29	MN	X	3013	1/1	0.95	0.25	70,70,70,70	0
29	MN	X	3436	1/1	0.95	0.17	119,119,119,119	0
30	MG	X	3451	1/1	0.95	0.30	115,115,115,115	0
29	MN	Y	202	1/1	0.95	0.15	105,105,105,105	0
30	MG	X	3261	1/1	0.95	0.23	91,91,91,91	0
29	MN	X	3095	1/1	0.95	0.20	79,79,79,79	0
30	MG	X	3476	1/1	0.95	0.15	64,64,64,64	0
29	MN	X	3096	1/1	0.95	0.38	100,100,100,100	0
29	MN	X	3100	1/1	0.95	0.25	96,96,96,96	0
30	MG	X	3482	1/1	0.95	0.26	90,90,90,90	0
29	MN	X	3074	1/1	0.95	0.52	113,113,113,113	0
29	MN	X	3103	1/1	0.95	0.21	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	MG	X	3277	1/1	0.95	0.62	97,97,97,97	0
30	MG	X	3331	1/1	0.95	0.36	86,86,86,86	0
29	MN	X	3223	1/1	0.95	0.17	119,119,119,119	0
29	MN	X	3062	1/1	0.95	0.14	87,87,87,87	0
29	MN	X	3171	1/1	0.95	0.21	114,114,114,114	0
29	MN	X	3325	1/1	0.95	0.16	187,187,187,187	0
29	MN	X	3189	1/1	0.95	0.07	154,154,154,154	0
29	MN	X	3330	1/1	0.95	0.15	104,104,104,104	0
29	MN	X	3120	1/1	0.95	0.21	166,166,166,166	0
29	MN	X	3089	1/1	0.96	0.14	113,113,113,113	0
29	MN	X	3046	1/1	0.96	0.29	91,91,91,91	0
29	MN	X	3093	1/1	0.96	0.22	81,81,81,81	0
30	MG	X	3389	1/1	0.96	0.37	94,94,94,94	0
30	MG	X	3442	1/1	0.96	0.16	71,71,71,71	0
29	MN	X	3068	1/1	0.96	0.35	94,94,94,94	0
30	MG	X	3218	1/1	0.96	0.18	75,75,75,75	0
29	MN	X	3070	1/1	0.96	0.33	129,129,129,129	0
29	MN	X	3021	1/1	0.96	0.21	91,91,91,91	0
29	MN	X	3097	1/1	0.96	0.26	109,109,109,109	0
30	MG	X	3227	1/1	0.96	0.71	95,95,95,95	0
29	MN	X	3220	1/1	0.96	0.08	103,103,103,103	0
29	MN	X	3049	1/1	0.96	0.30	93,93,93,93	0
29	MN	X	3052	1/1	0.96	0.31	90,90,90,90	0
30	MG	X	3278	1/1	0.96	0.23	82,82,82,82	0
29	MN	X	3102	1/1	0.96	0.56	124,124,124,124	0
29	MN	X	3054	1/1	0.96	0.35	97,97,97,97	0
29	MN	X	3160	1/1	0.96	0.15	100,100,100,100	0
30	MG	X	3284	1/1	0.96	0.17	72,72,72,72	0
29	MN	X	3029	1/1	0.96	0.39	69,69,69,69	0
29	MN	X	3131	1/1	0.96	0.23	126,126,126,126	0
29	MN	X	3392	1/1	0.96	0.11	89,89,89,89	0
30	MG	X	3141	1/1	0.96	0.24	85,85,85,85	0
30	MG	X	3289	1/1	0.96	0.24	110,110,110,110	0
29	MN	X	3401	1/1	0.96	0.13	104,104,104,104	0
30	MG	X	3143	1/1	0.96	0.44	59,59,59,59	0
29	MN	X	3081	1/1	0.96	0.28	109,109,109,109	0
29	MN	X	3135	1/1	0.96	0.15	115,115,115,115	0
29	MN	X	3312	1/1	0.96	0.26	115,115,115,115	0
29	MN	X	3313	1/1	0.96	0.10	117,117,117,117	0
30	MG	X	3431	1/1	0.96	0.38	55,55,55,55	0
29	MN	X	3015	1/1	0.96	0.09	80,80,80,80	0
29	MN	X	3140	1/1	0.96	0.12	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
29	MN	X	3016	1/1	0.96	0.12	75,75,75,75	0
30	MG	Y	209	1/1	0.96	0.91	153,153,153,153	0
29	MN	X	3134	1/1	0.97	0.17	121,121,121,121	0
29	MN	X	3020	1/1	0.97	0.28	107,107,107,107	0
30	MG	X	3414	1/1	0.97	0.18	89,89,89,89	0
30	MG	Y	201	1/1	0.97	0.28	66,66,66,66	0
29	MN	X	3200	1/1	0.97	0.19	123,123,123,123	0
29	MN	X	3172	1/1	0.97	0.14	114,114,114,114	0
29	MN	X	3105	1/1	0.97	0.19	97,97,97,97	0
29	MN	X	3206	1/1	0.97	0.07	95,95,95,95	0
30	MG	X	3364	1/1	0.97	0.73	83,83,83,83	0
29	MN	X	3108	1/1	0.97	0.19	89,89,89,89	0
29	MN	X	3078	1/1	0.97	0.44	111,111,111,111	0
30	MG	X	3426	1/1	0.97	0.25	104,104,104,104	0
29	MN	X	3035	1/1	0.97	0.23	74,74,74,74	0
30	MG	C	301	1/1	0.97	0.40	64,64,64,64	0
29	MN	X	3026	1/1	0.97	0.29	66,66,66,66	0
29	MN	X	3374	1/1	0.97	0.12	104,104,104,104	0
30	MG	X	3267	1/1	0.97	0.26	72,72,72,72	0
29	MN	X	3048	1/1	0.97	0.43	93,93,93,93	0
29	MN	X	3086	1/1	0.97	0.47	92,92,92,92	0
29	MN	X	3088	1/1	0.97	0.28	101,101,101,101	0
30	MG	X	3276	1/1	0.97	0.23	67,67,67,67	0
30	MG	X	3377	1/1	0.97	0.43	121,121,121,121	0
30	MG	X	3221	1/1	0.97	0.12	89,89,89,89	0
29	MN	X	3063	1/1	0.97	0.31	70,70,70,70	0
29	MN	X	3234	1/1	0.97	0.05	144,144,144,144	0
30	MG	X	3281	1/1	0.97	0.71	113,113,113,113	0
29	MN	X	3402	1/1	0.97	0.13	108,108,108,108	0
29	MN	X	3502	1/1	0.97	0.26	88,88,88,88	0
29	MN	X	3235	1/1	0.97	0.11	155,155,155,155	0
29	MN	X	3064	1/1	0.97	0.18	84,84,84,84	0
29	MN	X	3065	1/1	0.97	0.37	97,97,97,97	0
29	MN	X	3409	1/1	0.97	0.17	87,87,87,87	0
29	MN	X	3245	1/1	0.97	0.21	129,129,129,129	0
29	MN	X	3067	1/1	0.97	0.42	104,104,104,104	0
29	MN	X	3012	1/1	0.97	0.38	79,79,79,79	0
29	MN	X	3187	1/1	0.97	0.09	137,137,137,137	0
29	MN	X	3069	1/1	0.97	0.29	103,103,103,103	0
29	MN	X	3051	1/1	0.97	0.24	97,97,97,97	0
29	MN	X	3191	1/1	0.97	0.06	138,138,138,138	0
29	MN	X	3001	1/1	0.97	0.38	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	MG	X	3296	1/1	0.97	0.21	45,45,45,45	0
29	MN	X	3031	1/1	0.97	0.24	68,68,68,68	0
29	MN	X	3056	1/1	0.97	0.18	88,88,88,88	0
29	MN	X	3195	1/1	0.97	0.22	139,139,139,139	0
30	MG	X	3410	1/1	0.97	0.16	95,95,95,95	0
29	MN	X	3057	1/1	0.97	0.23	68,68,68,68	0
29	MN	X	3216	1/1	0.98	0.04	94,94,94,94	0
29	MN	X	3106	1/1	0.98	0.14	100,100,100,100	0
29	MN	X	3107	1/1	0.98	0.29	73,73,73,73	0
29	MN	X	3055	1/1	0.98	0.26	86,86,86,86	0
29	MN	X	3091	1/1	0.98	0.16	92,92,92,92	0
29	MN	X	3075	1/1	0.98	0.23	71,71,71,71	0
30	MG	X	3269	1/1	0.98	0.17	132,132,132,132	0
30	MG	X	3271	1/1	0.98	0.26	92,92,92,92	0
29	MN	X	3076	1/1	0.98	0.30	90,90,90,90	0
30	MG	X	3273	1/1	0.98	0.46	124,124,124,124	0
29	MN	X	3038	1/1	0.98	0.31	106,106,106,106	0
29	MN	X	3039	1/1	0.98	0.34	79,79,79,79	0
29	MN	X	3169	1/1	0.98	0.19	107,107,107,107	0
29	MN	X	3459	1/1	0.98	0.34	161,161,161,161	0
30	MG	X	3279	1/1	0.98	0.34	67,67,67,67	0
29	MN	X	3257	1/1	0.98	0.06	93,93,93,93	0
29	MN	X	3170	1/1	0.98	0.17	104,104,104,104	0
29	MN	X	3080	1/1	0.98	0.23	78,78,78,78	0
29	MN	X	3099	1/1	0.98	0.28	82,82,82,82	0
29	MN	X	3028	1/1	0.98	0.26	53,53,53,53	0
29	MN	X	3403	1/1	0.98	0.10	114,114,114,114	0
29	MN	X	3014	1/1	0.98	0.27	53,53,53,53	0
29	MN	X	3467	1/1	0.98	0.38	72,72,72,72	0
29	MN	X	3118	1/1	0.98	0.19	65,65,65,65	0
29	MN	X	3030	1/1	0.98	0.38	69,69,69,69	0
29	MN	X	3152	1/1	0.98	0.16	75,75,75,75	0
30	MG	X	3491	1/1	0.98	0.15	86,86,86,86	0
29	MN	X	3061	1/1	0.98	0.13	92,92,92,92	0
29	MN	X	3472	1/1	0.98	0.21	110,110,110,110	0
29	MN	X	3121	1/1	0.98	0.17	104,104,104,104	0
30	MG	X	3430	1/1	0.98	0.40	74,74,74,74	0
29	MN	X	3053	1/1	0.98	0.22	58,58,58,58	0
29	MN	X	3156	1/1	0.98	0.21	77,77,77,77	0
30	MG	X	3256	1/1	0.98	0.37	69,69,69,69	0
29	MN	X	3022	1/1	0.98	0.11	92,92,92,92	0
29	MN	X	3503	1/1	0.98	0.25	68,68,68,68	0

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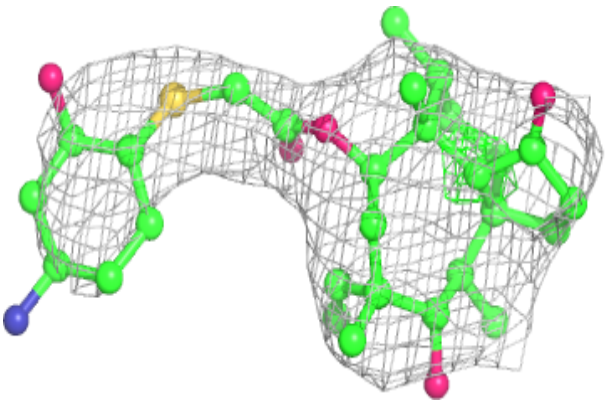
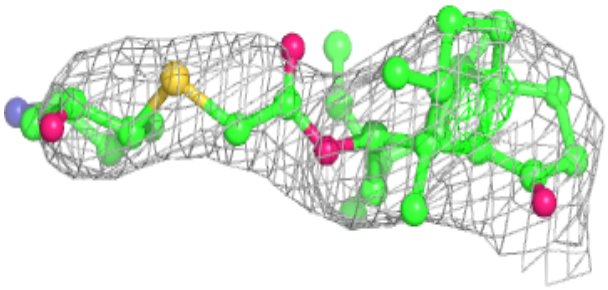
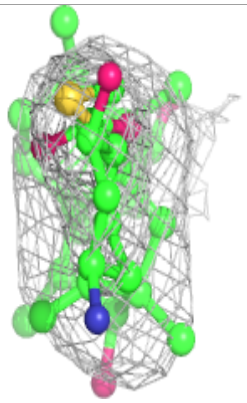
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
29	MN	X	3042	1/1	0.99	0.23	74,74,74,74	0
29	MN	X	3132	1/1	0.99	0.20	104,104,104,104	0
29	MN	X	3079	1/1	0.99	0.27	58,58,58,58	0
29	MN	X	3092	1/1	0.99	0.22	90,90,90,90	0
29	MN	X	3457	1/1	0.99	0.45	135,135,135,135	0
29	MN	X	3251	1/1	0.99	0.12	81,81,81,81	0
29	MN	X	3043	1/1	0.99	0.34	81,81,81,81	0
29	MN	X	3136	1/1	0.99	0.25	55,55,55,55	0
29	MN	X	3201	1/1	0.99	0.15	88,88,88,88	0
29	MN	X	3050	1/1	0.99	0.25	98,98,98,98	0
29	MN	X	3270	1/1	0.99	0.12	110,110,110,110	0
29	MN	X	3032	1/1	0.99	0.33	64,64,64,64	0
29	MN	X	3145	1/1	0.99	0.19	69,69,69,69	0
29	MN	X	3083	1/1	0.99	0.31	73,73,73,73	0
29	MN	X	3164	1/1	0.99	0.28	111,111,111,111	0
29	MN	X	3066	1/1	0.99	0.24	80,80,80,80	0
29	MN	X	3098	1/1	0.99	0.19	92,92,92,92	0
30	MG	X	3275	1/1	0.99	0.16	71,71,71,71	0
29	MN	X	3215	1/1	0.99	0.14	87,87,87,87	0
29	MN	X	3188	1/1	0.99	0.25	114,114,114,114	0
29	MN	X	3217	1/1	0.99	0.14	86,86,86,86	0
29	MN	X	3219	1/1	0.99	0.15	85,85,85,85	0
29	MN	X	3033	1/1	0.99	0.27	78,78,78,78	0
29	MN	X	3040	1/1	0.99	0.36	81,81,81,81	0
29	MN	X	3126	1/1	0.99	0.21	74,74,74,74	0
29	MN	X	3127	1/1	0.99	0.17	94,94,94,94	0
29	MN	X	3023	1/1	0.99	0.27	92,92,92,92	0
29	MN	X	3018	1/1	1.00	0.12	86,86,86,86	0
29	MN	X	3085	1/1	1.00	0.27	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.

Electron density around 62B X 3003: 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 (i)

There are no such residues in this entry.