



wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 11:35 pm BST

PDB ID : 5HKV
Title : The crystal structure of the large ribosomal subunit of *Staphylococcus aureus* in complex with lincomycin
Authors : Yonath, A.; Matzov, D.; Eyal, Z.; Ben Hamou, R.; Zimmerman, E.; Rozenberg, H.; Bashan, A.; Fridman, M.
Deposited on : 2016-01-14
Resolution : 3.66 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

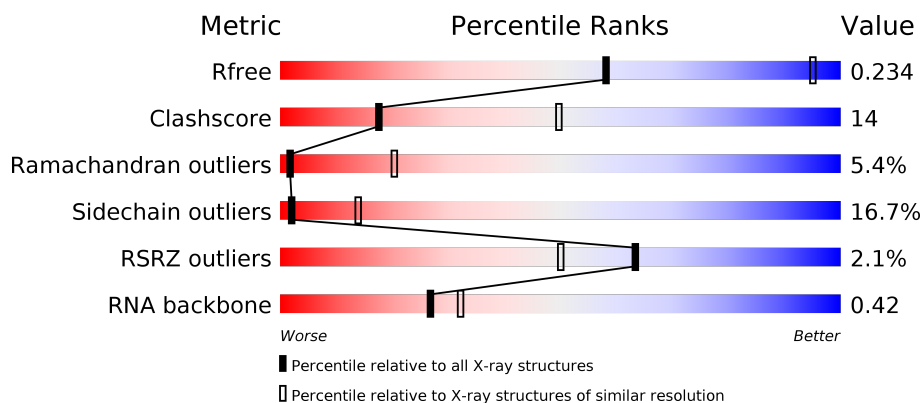
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.66 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.














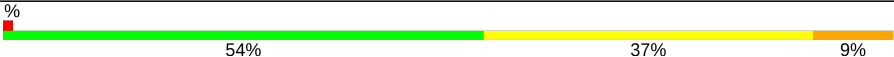

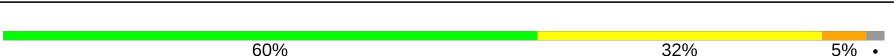
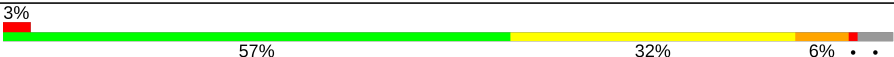

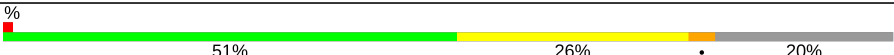
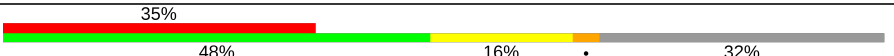
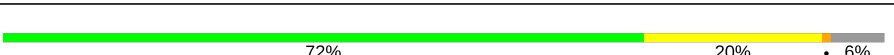
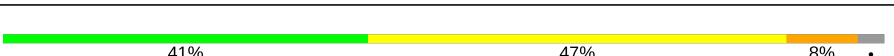
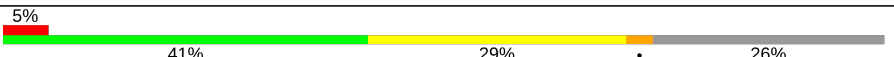


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1557 (3.82-3.50)
Clashscore	141614	1037 (3.80-3.52)
Ramachandran outliers	138981	1004 (3.80-3.52)
Sidechain outliers	138945	1002 (3.80-3.52)
RSRZ outliers	127900	1441 (3.82-3.50)
RNA backbone	3102	1024 (4.30-3.00)

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

Mol	Chain	Length	Quality of chain
1	X	2923	<div> <div>34%</div> <div>40%</div> <div>16%</div> <div>8%</div> </div>
2	Y	114	<div> <div>43%</div> <div>40%</div> <div>16%</div> </div>
3	A	277	<div> <div>3%</div> <div>69%</div> <div>23%</div> <div>5%</div> </div>
4	B	220	<div> <div>59%</div> <div>35%</div> </div>

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Mol	Chain	Length	Quality of chain
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	

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	MPD	X	3024	-	-	-	X
30	MN	A	304	-	-	-	X
30	MN	X	3028	-	-	-	X
30	MN	X	3031	-	-	-	X
30	MN	X	3032	-	-	-	X
30	MN	X	3052	-	-	-	X
30	MN	X	3087	-	-	-	X
30	MN	X	3117	-	-	-	X
30	MN	X	3178	-	-	-	X
30	MN	X	3214	-	-	-	X
30	MN	X	3254	-	-	-	X
30	MN	X	3288	-	-	-	X
30	MN	X	3343	-	-	-	X
30	MN	X	3345	-	-	-	X
30	MN	X	3346	-	-	-	X
30	MN	X	3354	-	-	-	X
30	MN	X	3358	-	-	-	X
30	MN	X	3365	-	-	-	X
30	MN	X	3376	-	-	-	X
30	MN	X	3381	-	-	-	X
30	MN	X	3382	-	-	-	X
30	MN	X	3383	-	-	-	X
30	MN	X	3397	-	-	-	X
30	MN	X	3398	-	-	-	X
30	MN	X	3399	-	-	-	X
30	MN	X	3410	-	-	-	X
30	MN	X	3413	-	-	-	X
30	MN	X	3430	-	-	-	X
30	MN	X	3431	-	-	-	X
30	MN	Y	211	-	-	-	X
30	MN	Z	101	-	-	-	X
31	MG	B	301	-	-	-	X
31	MG	G	203	-	-	-	X
31	MG	L	201	-	-	-	X
31	MG	P	202	-	-	-	X
31	MG	S	302	-	-	-	X
31	MG	X	3071	-	-	-	X
31	MG	X	3073	-	-	-	X
31	MG	X	3074	-	-	-	X
31	MG	X	3077	-	-	-	X
31	MG	X	3089	-	-	-	X
31	MG	X	3090	-	-	-	X
31	MG	X	3103	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	MG	X	3106	-	-	-	X
31	MG	X	3108	-	-	-	X
31	MG	X	3109	-	-	-	X
31	MG	X	3450	-	-	-	X
31	MG	X	3461	-	-	-	X
32	SPD	X	3489	-	-	X	-
32	SPD	Y	213	-	-	-	X
33	EOH	C	303	-	-	X	-
33	EOH	R	203	-	-	X	-
33	EOH	X	3491	-	-	-	X
33	EOH	X	3495	-	-	-	X

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 80892 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 ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	2695	Total	C	N	O	P	0	0	0
			57765	25787	10584	18699	2695			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	269	Total	C	N	O	S	0	0	0
			1643	992	326	320	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	215	Total	C	N	O	S	0	0	0
			1551	972	290	284	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	199	Total	C	N	O	S	0	0	0
			1314	815	249	248	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	166	Total	C	N	O	S	0	0	0
			857	517	166	173	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	158	Total	C	N	O	S	0	0	0
			942	569	177	194	2			

- 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
			1088	682	201	203	2			

- 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
			880	545	166	165	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
			794	480	162	152				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	137	Total	C	N	O	S	0	0	0
			919	591	165	161	2			

- 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
			888	544	172	171	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	L	109	Total	C	N	O	S	0	0	0
			677	415	130	132				

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	M	108	Total	C	N	O			
			796	505	156	135	0	0	0

- 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			
			913	574	183	152	4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	O	102	Total	C	N	O	S			
			743	472	137	133	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	P	112	Total	C	N	O	S			
			841	526	159	153	3	0	0	0

- 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			
			600	374	107	116	3	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	R	101	Total	C	N	O	S			
			592	358	111	122	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	S	167	Total	C	N	O	S			
			1097	690	191	214	2	0	0	0

- 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
			526	325	102	99			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	U	42	Total	C	N	O	0	0	0
			235	146	46	43			

- 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
			466	288	81	97			

- 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
			441	274	83	84			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Z	43	Total	C	N	O	S	0	0	0
			328	200	69	55	4			

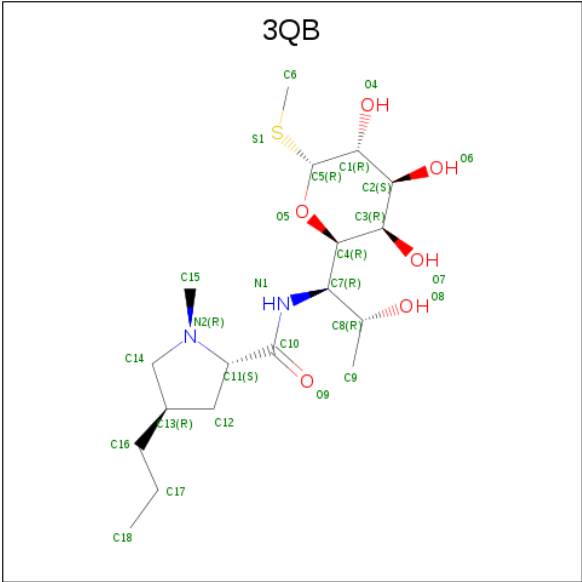
- Molecule 26 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	2	44	Total	C	N	O	S	0	0	0
			328	198	76	53	1			

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

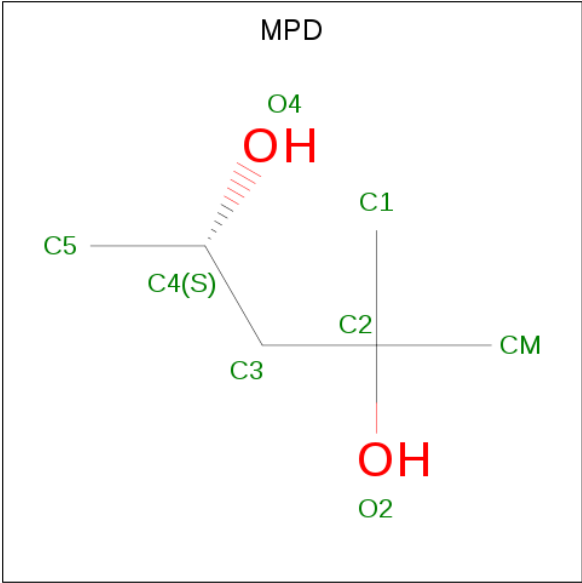
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	3	60	Total	C	N	O	S	0	0	0
			401	246	80	73	2			

- Molecule 28 is LINCOMYCIN (three-letter code: 3QB) (formula: C₁₈H₃₄N₂O₆S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
28	X	1	Total	C	N	O	S	0	0
			27	18	2	6	1		

- Molecule 29 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C₆H₁₄O₂).



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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	S	1	Total	C	O	0	0
			8	6	2		

- Molecule 30 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	J	2	Total	Mn	0	0
			2	2		
30	I	1	Total	Mn	0	0
			1	1		
30	C	2	Total	Mn	0	0
			2	2		
30	Z	1	Total	Mn	0	0
			1	1		
30	A	2	Total	Mn	0	0
			2	2		
30	N	1	Total	Mn	0	0
			1	1		
30	X	319	Total	Mn	0	0
			319	319		
30	R	1	Total	Mn	0	0
			1	1		
30	Y	8	Total	Mn	0	0
			8	8		
30	S	1	Total	Mn	0	0
			1	1		

- Molecule 31 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

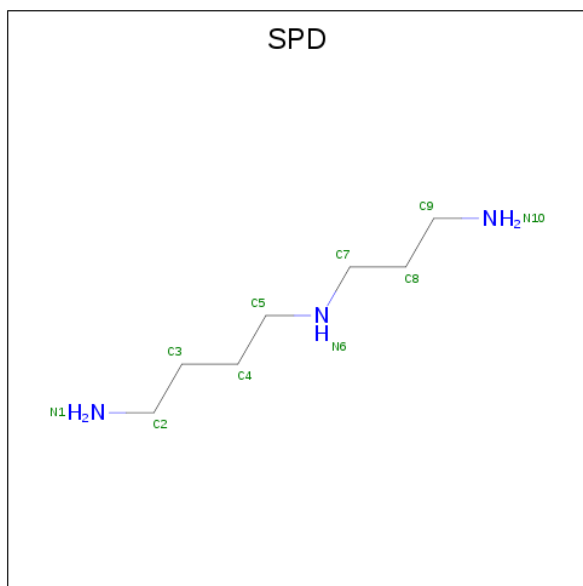
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
31	P	2	Total	Mg	0	0
			2	2		
31	G	3	Total	Mg	0	0
			3	3		
31	K	1	Total	Mg	0	0
			1	1		
31	B	1	Total	Mg	0	0
			1	1		
31	3	2	Total	Mg	0	0
			2	2		
31	A	3	Total	Mg	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
31	T	1	Total	Mg	0	0
			1	1		
31	2	1	Total	Mg	0	0
			1	1		
31	X	140	Total	Mg	0	0
			140	140		
31	O	1	Total	Mg	0	0
			1	1		
31	R	1	Total	Mg	0	0
			1	1		
31	Y	3	Total	Mg	0	0
			3	3		
31	L	1	Total	Mg	0	0
			1	1		
31	S	1	Total	Mg	0	0
			1	1		
31	M	1	Total	Mg	0	0
			1	1		

- Molecule 32 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



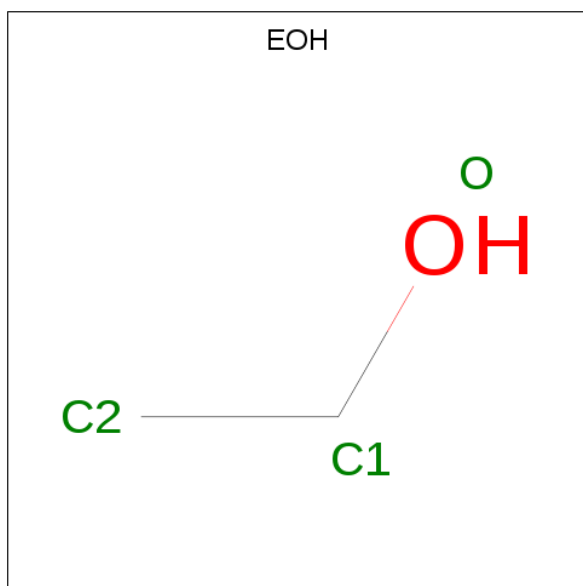
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	X	1	Total	C	N	0	0
			10	7	3		
32	X	1	Total	C	N	0	0
			10	7	3		

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

- Molecule 33 is ETHANOL (three-letter code: EOH) (formula: C_2H_6O).



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

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

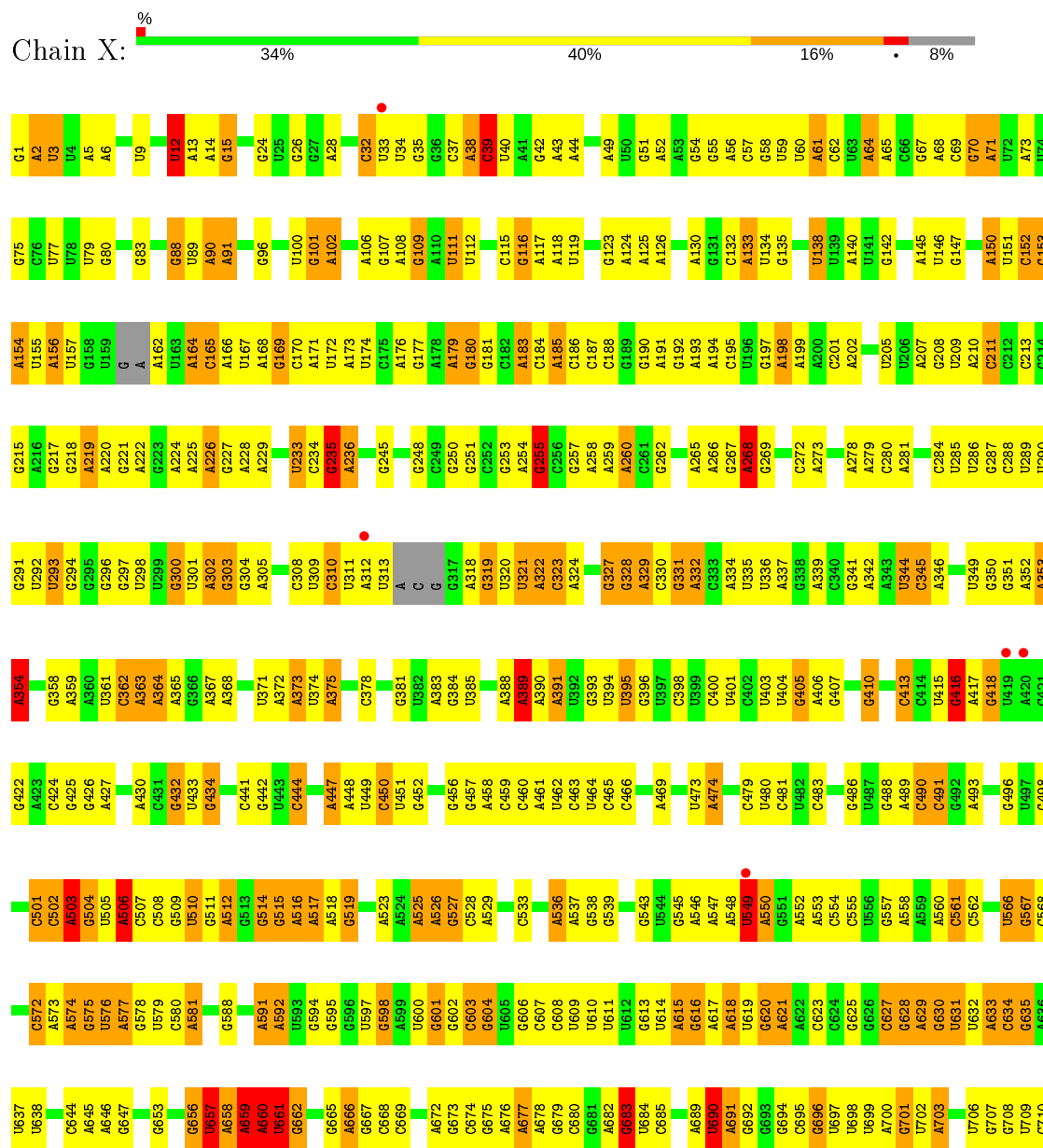
- Molecule 34 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	Y	1	Total	Ca	0	0
			1	1		

3 Residue-property plots

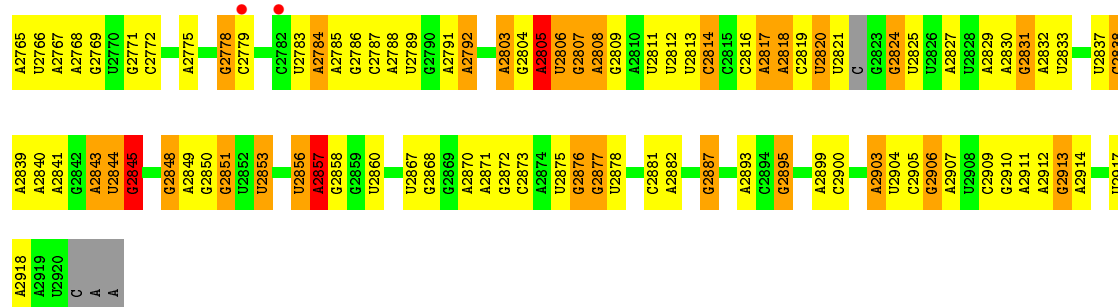
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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



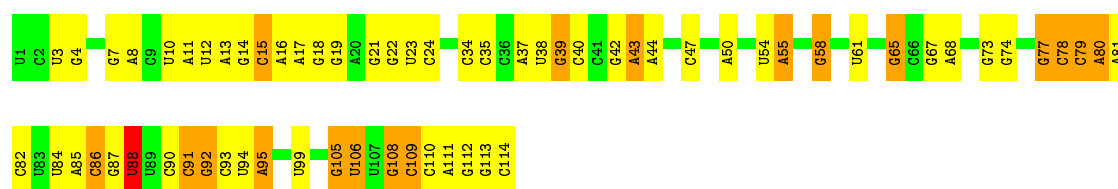






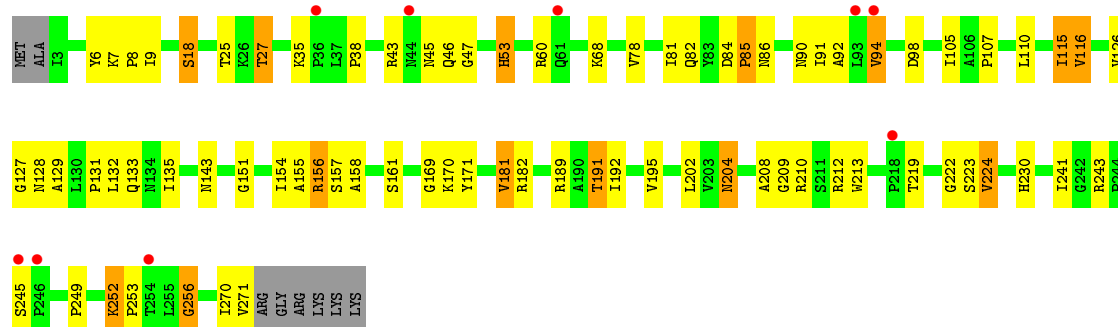
- Molecule 2: 5S ribosomal RNA

Chain Y: 43% 40% 16% .



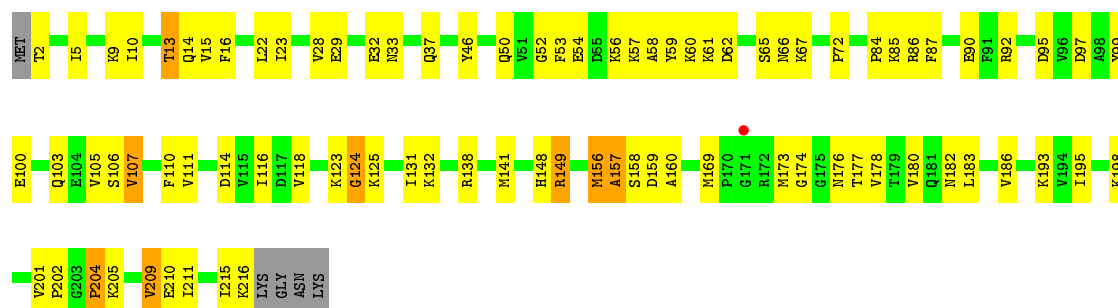
- Molecule 3: 50S ribosomal protein L2

Chain A: 3% 69% 23% 5% .

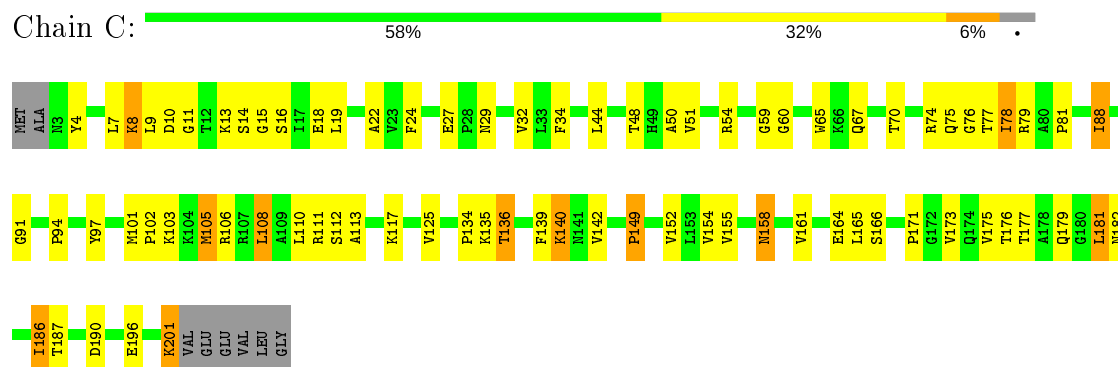


- Molecule 4: 50S ribosomal protein L3

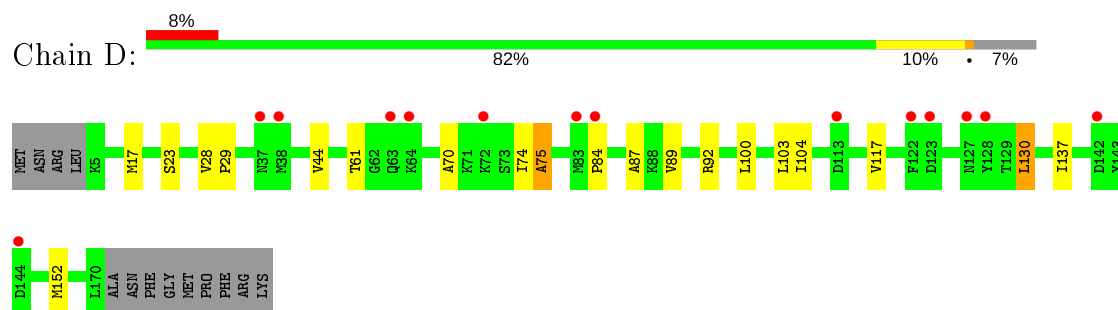
Chain B: 59% 35% . .



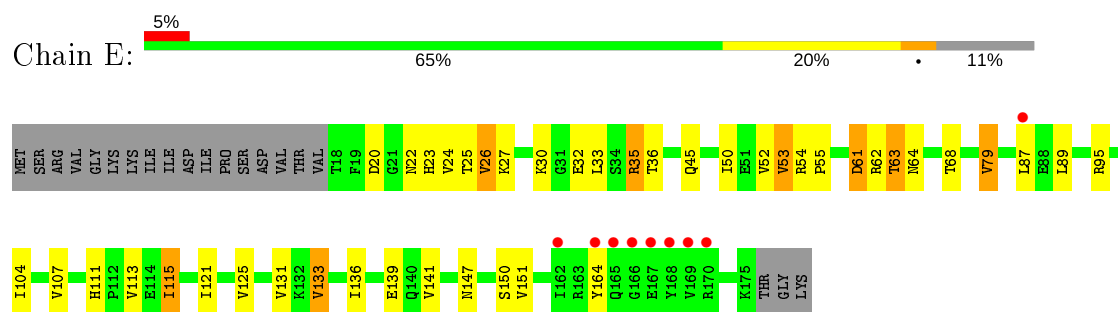
- Molecule 5: 50S ribosomal protein L4



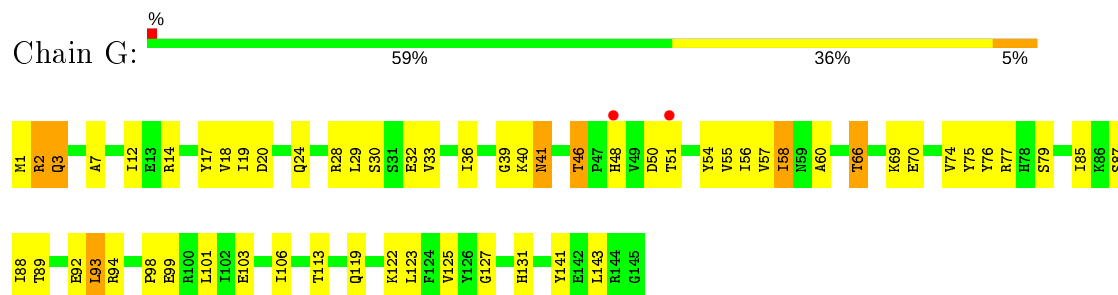
- Molecule 6: 50S ribosomal protein L5



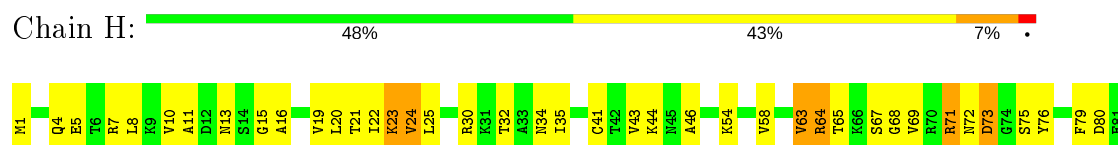
- Molecule 7: 50S ribosomal protein L6



- Molecule 8: 50S ribosomal protein L13



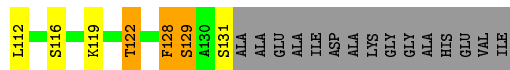
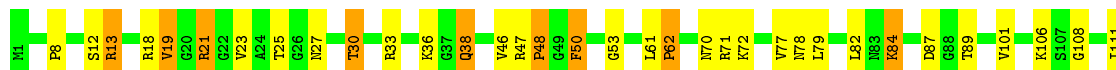
- Molecule 9: 50S ribosomal protein L14





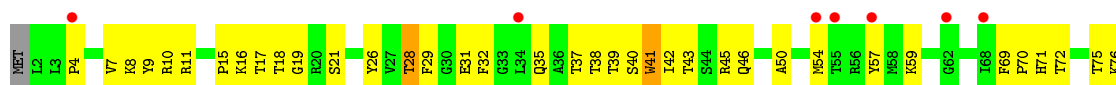
- Molecule 10: 50S ribosomal protein L15

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:



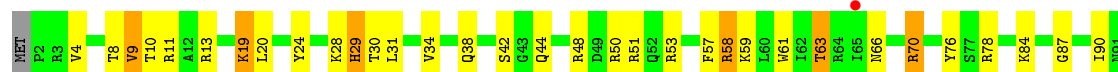
- Molecule 14: 50S ribosomal protein L19

Chain M:

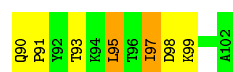




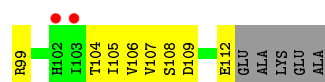
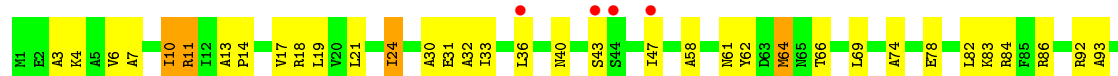
• Molecule 15: 50S ribosomal protein L20



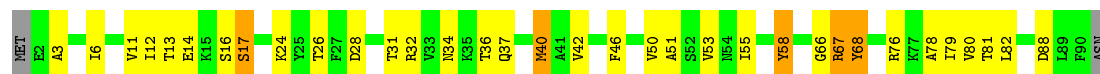
• Molecule 16: 50S ribosomal protein L21



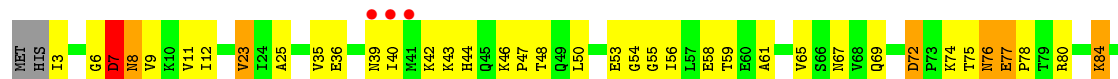
• Molecule 17: 50S ribosomal protein L22



• Molecule 18: 50S ribosomal protein L23

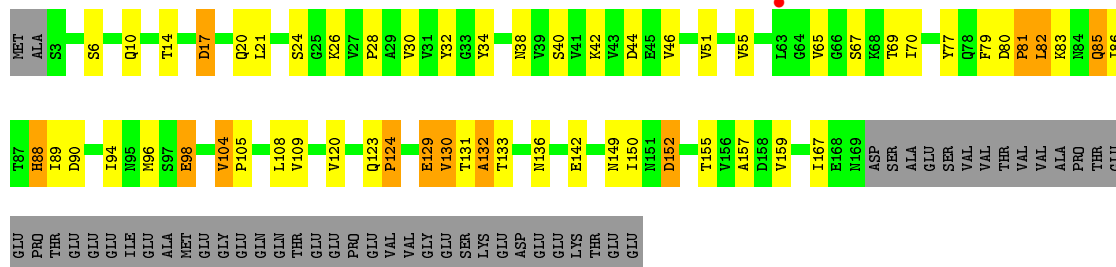


• Molecule 19: 50S ribosomal protein L24

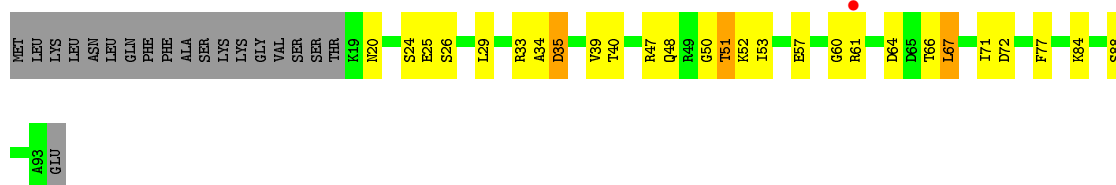




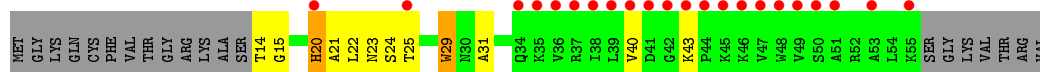
- Molecule 20: 50S ribosomal protein L25



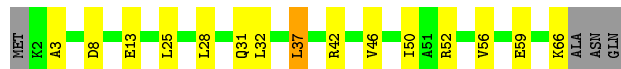
- Molecule 21: 50S ribosomal protein L27



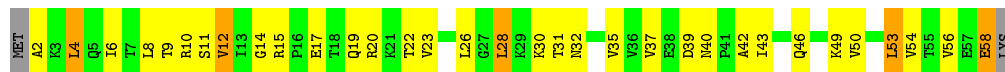
- Molecule 22: 50S ribosomal protein L28



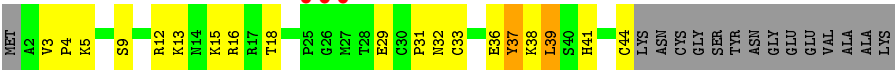
- Molecule 23: 50S ribosomal protein L29



- Molecule 24: 50S ribosomal protein L30



- Molecule 25: 50S ribosomal protein L32



• Molecule 26: 50S ribosomal protein L34



• Molecule 27: 50S ribosomal protein L35



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	280.88Å 280.88Å 873.52Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.66 69.74 – 3.66	Depositor EDS
% Data completeness (in resolution range)	98.2 (50.00-3.66) 98.2 (69.74-3.66)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 3.67Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.187 , 0.234 0.188 , 0.234	Depositor DCC
R_{free} test set	10832 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	124.9	Xtriage
Anisotropy	0.213	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 83.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	80892	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.89	60/64681 (0.1%)	1.45	879/100838 (0.9%)
2	Y	0.76	1/2717 (0.0%)	1.41	46/4232 (1.1%)
3	A	0.28	0/1672	0.56	0/2302
4	B	0.41	0/1574	0.67	0/2121
5	C	0.40	0/1332	0.63	0/1822
6	D	0.29	0/859	0.53	0/1192
7	E	0.43	0/947	0.61	0/1303
8	G	0.40	0/1110	0.62	0/1505
9	H	0.58	1/887 (0.1%)	0.80	1/1199 (0.1%)
10	I	0.43	0/801	0.72	0/1089
11	J	0.57	0/941	0.80	0/1289
12	K	0.69	0/891	0.91	0/1196
13	L	0.28	0/682	0.51	0/933
14	M	0.61	0/808	0.79	0/1094
15	N	0.45	0/925	0.64	0/1232
16	O	0.63	0/753	0.90	2/1013 (0.2%)
17	P	0.72	0/849	0.93	0/1147
18	Q	0.51	0/606	0.74	0/828
19	R	0.31	0/594	0.65	0/814
20	S	0.52	0/1109	0.82	1/1522 (0.1%)
21	T	0.55	0/532	0.79	0/714
22	U	0.39	0/240	0.64	0/335
23	V	0.50	0/467	0.68	0/631
24	W	0.73	0/443	0.88	0/597
25	Z	0.67	0/333	0.81	0/444
26	2	0.56	0/331	0.74	0/441
27	3	0.72	0/405	0.96	0/545
All	All	0.82	62/87489 (0.1%)	1.33	929/132378 (0.7%)

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
3	A	0	1
11	J	0	1
20	S	0	1
21	T	0	1
22	U	0	1
27	3	0	2
All	All	0	7

The worst 5 of 62 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	1289	A	N9-C4	-11.33	1.31	1.37
1	X	1186	A	N9-C4	-9.86	1.31	1.37
1	X	2087	A	N9-C4	-8.21	1.32	1.37
1	X	865	A	N9-C4	-7.63	1.33	1.37
1	X	518	A	N9-C4	-7.24	1.33	1.37

The worst 5 of 929 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1746	G	C8-N9-C4	-14.62	100.55	106.40
1	X	2845	G	N3-C4-N9	-14.02	117.59	126.00
1	X	2845	G	N3-C4-C5	13.93	135.56	128.60
1	X	1229	G	C5-C6-O6	-12.16	121.30	128.60
2	Y	93	C	N3-C2-O2	-12.10	113.43	121.90

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	115	ILE	Peptide
11	J	8	LYS	Peptide
20	S	17	ASP	Peptide
21	T	25	GLU	Peptide
22	U	43	LYS	Peptide

5.2 Too-close contacts ⓘ

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	57765	0	29049	1096	0
2	Y	2430	0	1229	47	0
3	A	1643	0	1245	42	0
4	B	1551	0	1532	54	0
5	C	1314	0	1159	46	0
6	D	857	0	453	11	0
7	E	942	0	693	18	0
8	G	1088	0	1035	35	0
9	H	880	0	891	62	0
10	I	794	0	630	26	0
11	J	919	0	806	38	0
12	K	888	0	891	65	0
13	L	677	0	543	9	0
14	M	796	0	794	36	0
15	N	913	0	949	32	0
16	O	743	0	728	30	0
17	P	841	0	874	37	0
18	Q	600	0	509	26	0
19	R	592	0	436	21	0
20	S	1097	0	956	29	0
21	T	526	0	488	16	0
22	U	235	0	128	8	0
23	V	466	0	430	8	0
24	W	441	0	478	27	0
25	Z	328	0	318	17	0
26	2	328	0	325	10	0
27	3	401	0	357	16	0
28	X	27	0	34	3	0
29	S	8	0	14	0	0
29	X	184	0	322	20	0
30	A	2	0	0	0	0
30	C	2	0	0	0	0
30	I	1	0	0	0	0
30	J	2	0	0	0	0
30	N	1	0	0	0	0
30	R	1	0	0	0	0
30	S	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	X	319	0	0	0	0
30	Y	8	0	0	0	0
30	Z	1	0	0	0	0
31	2	1	0	0	0	0
31	3	2	0	0	0	0
31	A	3	0	0	0	0
31	B	1	0	0	0	0
31	G	3	0	0	0	0
31	K	1	0	0	0	0
31	L	1	0	0	0	0
31	M	1	0	0	0	0
31	O	1	0	0	0	0
31	P	2	0	0	0	0
31	R	1	0	0	0	0
31	S	1	0	0	0	0
31	T	1	0	0	0	0
31	X	140	0	0	0	0
31	Y	3	0	0	0	0
32	X	80	0	152	20	0
32	Y	10	0	19	0	0
33	C	3	0	6	2	0
33	R	3	0	6	2	0
33	X	21	0	42	1	0
34	Y	1	0	0	0	0
All	All	80892	0	48521	1698	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 14.

The worst 5 of 1698 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)
9:H:98:ILE:HB	9:H:118:ALA:HB2	1.30	1.12
9:H:98:ILE:HG12	9:H:117:LEU:CD1	1.81	1.10
9:H:98:ILE:HG12	9:H:117:LEU:HD12	1.33	1.08
1:X:2231:C:HO2'	1:X:2232:A:H8	1.07	0.96
1:X:1487:G:N2	1:X:1597:U:O2	2.01	0.92

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	267/277 (96%)	216 (81%)	31 (12%)	20 (8%)	1	13
4	B	213/220 (97%)	185 (87%)	17 (8%)	11 (5%)	2	21
5	C	197/207 (95%)	168 (85%)	20 (10%)	9 (5%)	2	23
6	D	164/179 (92%)	141 (86%)	15 (9%)	8 (5%)	2	22
7	E	156/178 (88%)	121 (78%)	23 (15%)	12 (8%)	1	12
8	G	143/145 (99%)	132 (92%)	7 (5%)	4 (3%)	5	33
9	H	120/122 (98%)	105 (88%)	11 (9%)	4 (3%)	4	31
10	I	129/146 (88%)	94 (73%)	23 (18%)	12 (9%)	0	9
11	J	135/144 (94%)	115 (85%)	12 (9%)	8 (6%)	1	18
12	K	117/122 (96%)	103 (88%)	6 (5%)	8 (7%)	1	15
13	L	107/119 (90%)	91 (85%)	14 (13%)	2 (2%)	8	40
14	M	106/116 (91%)	92 (87%)	7 (7%)	7 (7%)	1	16
15	N	114/118 (97%)	109 (96%)	3 (3%)	2 (2%)	8	41
16	O	100/102 (98%)	90 (90%)	6 (6%)	4 (4%)	3	26
17	P	110/117 (94%)	103 (94%)	7 (6%)	0	100	100
18	Q	87/91 (96%)	72 (83%)	12 (14%)	3 (3%)	3	30
19	R	99/105 (94%)	75 (76%)	13 (13%)	11 (11%)	0	5
20	S	165/217 (76%)	125 (76%)	25 (15%)	15 (9%)	1	9
21	T	73/94 (78%)	61 (84%)	9 (12%)	3 (4%)	3	25
22	U	40/62 (64%)	36 (90%)	2 (5%)	2 (5%)	2	22
23	V	63/69 (91%)	57 (90%)	4 (6%)	2 (3%)	4	31
24	W	55/59 (93%)	53 (96%)	2 (4%)	0	100	100
25	Z	41/58 (71%)	39 (95%)	1 (2%)	1 (2%)	6	35
26	2	42/45 (93%)	38 (90%)	3 (7%)	1 (2%)	6	35
27	3	58/66 (88%)	42 (72%)	9 (16%)	7 (12%)	0	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2901/3178 (91%)	2463 (85%)	282 (10%)	156 (5%)	2	20

5 of 156 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	27	THR
3	A	35	LYS
3	A	38	PRO
3	A	126	VAL
3	A	192	ILE

5.3.2 Protein sidechains ⓘ

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	106/224 (47%)	91 (86%)	15 (14%)	3	19
4	B	151/177 (85%)	139 (92%)	12 (8%)	12	42
5	C	103/169 (61%)	80 (78%)	23 (22%)	1	6
6	D	15/158 (10%)	13 (87%)	2 (13%)	4	21
7	E	59/155 (38%)	48 (81%)	11 (19%)	1	10
8	G	106/123 (86%)	96 (91%)	10 (9%)	8	35
9	H	90/100 (90%)	75 (83%)	15 (17%)	2	14
10	I	48/112 (43%)	35 (73%)	13 (27%)	0	3
11	J	71/119 (60%)	58 (82%)	13 (18%)	1	10
12	K	86/102 (84%)	64 (74%)	22 (26%)	0	4
13	L	42/95 (44%)	32 (76%)	10 (24%)	0	5
14	M	76/102 (74%)	58 (76%)	18 (24%)	1	5
15	N	88/98 (90%)	77 (88%)	11 (12%)	4	23
16	O	69/86 (80%)	55 (80%)	14 (20%)	1	8
17	P	84/94 (89%)	77 (92%)	7 (8%)	11	40
18	Q	47/82 (57%)	34 (72%)	13 (28%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	R	35/90 (39%)	24 (69%)	11 (31%)	0	2
20	S	91/190 (48%)	78 (86%)	13 (14%)	3	19
21	T	45/75 (60%)	37 (82%)	8 (18%)	2	11
22	U	5/52 (10%)	3 (60%)	2 (40%)	0	0
23	V	43/62 (69%)	39 (91%)	4 (9%)	9	36
24	W	51/53 (96%)	41 (80%)	10 (20%)	1	8
25	Z	33/51 (65%)	29 (88%)	4 (12%)	5	24
26	2	30/40 (75%)	28 (93%)	2 (7%)	16	48
27	3	32/57 (56%)	27 (84%)	5 (16%)	2	16
All	All	1606/2666 (60%)	1338 (83%)	268 (17%)	2	14

5 of 268 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	K	41	ARG
14	M	17	THR
24	W	4	LEU
12	K	65	THR
13	L	11	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
4	B	148	HIS
11	J	123	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2675/2923 (91%)	659 (24%)	27 (1%)
2	Y	113/114 (99%)	17 (15%)	0
All	All	2788/3037 (91%)	676 (24%)	27 (0%)

5 of 676 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	2	A

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Mol	Chain	Res	Type
1	X	3	U
1	X	12	U
1	X	15	G
1	X	34	U

5 of 27 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	1091	G
1	X	1503	U
1	X	2062	G
1	X	1250	G
1	X	184	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 544 ligands modelled in this entry, 501 are monoatomic - leaving 43 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	EOH	C	303	-	2,2,2	0.54	0	1,1,1	0.38	0
29	MPD	X	3012	-	7,7,7	0.40	0	9,10,10	0.15	0
32	SPD	X	3489	-	9,9,9	0.14	0	8,8,8	0.23	0
29	MPD	X	3019	-	7,7,7	1.30	1 (14%)	9,10,10	0.44	0
32	SPD	Y	213	-	9,9,9	0.25	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	EOH	X	3495	-	2,2,2	0.57	0	1,1,1	0.67	0
33	EOH	R	203	-	2,2,2	0.32	0	1,1,1	0.40	0
29	MPD	X	3014	-	7,7,7	0.87	1 (14%)	9,10,10	0.44	0
33	EOH	X	3492	-	2,2,2	0.76	0	1,1,1	0.13	0
29	MPD	X	3013	-	7,7,7	0.81	0	9,10,10	0.44	0
32	SPD	X	3485	-	9,9,9	0.19	0	8,8,8	0.25	0
29	MPD	X	3002	-	7,7,7	0.53	0	9,10,10	0.26	0
29	MPD	X	3017	-	7,7,7	0.78	0	9,10,10	0.36	0
33	EOH	X	3491	-	2,2,2	0.58	0	1,1,1	0.62	0
33	EOH	X	3490	-	2,2,2	0.56	0	1,1,1	0.50	0
29	MPD	X	3016	-	7,7,7	0.68	0	9,10,10	0.16	0
29	MPD	X	3018	-	7,7,7	0.97	1 (14%)	9,10,10	0.43	0
32	SPD	X	3487	-	9,9,9	0.11	0	8,8,8	0.24	0
29	MPD	X	3011	-	7,7,7	0.55	0	9,10,10	0.36	0
29	MPD	S	301	-	7,7,7	0.77	0	9,10,10	0.30	0
29	MPD	X	3020	-	7,7,7	0.71	0	9,10,10	0.33	0
32	SPD	X	3484	-	9,9,9	0.16	0	8,8,8	0.38	0
32	SPD	X	3486	-	9,9,9	0.29	0	8,8,8	0.35	0
33	EOH	X	3493	-	2,2,2	0.56	0	1,1,1	0.55	0
29	MPD	X	3008	-	7,7,7	0.73	0	9,10,10	0.42	0
29	MPD	X	3010	-	7,7,7	0.53	0	9,10,10	0.31	0
29	MPD	X	3021	-	7,7,7	0.95	1 (14%)	9,10,10	0.52	0
29	MPD	X	3009	-	7,7,7	0.67	0	9,10,10	0.22	0
29	MPD	X	3007	-	7,7,7	0.69	0	9,10,10	0.50	0
29	MPD	X	3022	-	7,7,7	1.16	1 (14%)	9,10,10	0.48	0
29	MPD	X	3004	-	7,7,7	0.72	0	9,10,10	0.19	0
33	EOH	X	3496	-	2,2,2	0.63	0	1,1,1	0.43	0
29	MPD	X	3023	-	7,7,7	0.92	1 (14%)	9,10,10	0.60	0
29	MPD	X	3005	-	7,7,7	0.92	1 (14%)	9,10,10	0.54	0
28	3QB	X	3001	-	25,28,28	0.95	2 (8%)	29,40,40	1.25	3 (10%)
29	MPD	X	3024	-	7,7,7	0.94	1 (14%)	9,10,10	0.23	0
32	SPD	X	3483	-	9,9,9	0.25	0	8,8,8	0.47	0
29	MPD	X	3015	-	7,7,7	0.54	0	9,10,10	0.33	0
29	MPD	X	3006	-	7,7,7	0.62	0	9,10,10	0.37	0
33	EOH	X	3494	-	2,2,2	0.42	0	1,1,1	0.78	0
29	MPD	X	3003	-	7,7,7	0.85	0	9,10,10	0.49	0
32	SPD	X	3488	-	9,9,9	0.26	0	8,8,8	0.39	0
32	SPD	X	3482	-	9,9,9	0.19	0	8,8,8	0.20	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
29	MPD	X	3012	-	-	5/5/5/5	-
32	SPD	X	3489	-	-	2/7/7/7	-
29	MPD	X	3019	-	-	0/5/5/5	-
32	SPD	Y	213	-	-	2/7/7/7	-
32	SPD	X	3484	-	-	3/7/7/7	-
29	MPD	X	3014	-	-	0/5/5/5	-
29	MPD	X	3013	-	-	0/5/5/5	-
32	SPD	X	3485	-	-	1/7/7/7	-
29	MPD	X	3002	-	-	1/5/5/5	-
29	MPD	X	3017	-	-	1/5/5/5	-
29	MPD	X	3016	-	-	1/5/5/5	-
29	MPD	X	3018	-	-	0/5/5/5	-
32	SPD	X	3487	-	-	1/7/7/7	-
29	MPD	X	3011	-	-	1/5/5/5	-
29	MPD	S	301	-	-	3/5/5/5	-
29	MPD	X	3020	-	-	0/5/5/5	-
32	SPD	X	3486	-	-	4/7/7/7	-
29	MPD	X	3008	-	-	1/5/5/5	-
29	MPD	X	3010	-	-	0/5/5/5	-
29	MPD	X	3021	-	-	0/5/5/5	-
29	MPD	X	3009	-	-	3/5/5/5	-
29	MPD	X	3007	-	-	1/5/5/5	-
29	MPD	X	3022	-	-	2/5/5/5	-
29	MPD	X	3004	-	-	2/5/5/5	-
29	MPD	X	3023	-	-	3/5/5/5	-
29	MPD	X	3005	-	-	4/5/5/5	-
28	3QB	X	3001	-	-	10/21/53/53	0/2/2/2
29	MPD	X	3024	-	-	1/5/5/5	-
32	SPD	X	3483	-	-	4/7/7/7	-
29	MPD	X	3015	-	-	3/5/5/5	-
29	MPD	X	3006	-	-	1/5/5/5	-
29	MPD	X	3003	-	-	5/5/5/5	-
32	SPD	X	3488	-	-	3/7/7/7	-
32	SPD	X	3482	-	-	2/7/7/7	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	X	3019	MPD	C3-C2	3.07	1.62	1.53
29	X	3022	MPD	C3-C2	2.72	1.61	1.53
28	X	3001	3QB	C7-N1	-2.66	1.41	1.45
28	X	3001	3QB	C11-C10	-2.49	1.47	1.52
29	X	3018	MPD	C3-C2	2.27	1.59	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	X	3001	3QB	C7-N1-C10	3.88	129.07	123.21
28	X	3001	3QB	C12-C11-N2	-2.45	98.55	103.88
28	X	3001	3QB	O9-C10-N1	-2.35	118.58	122.93

There are no chirality outliers.

5 of 70 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	X	3005	MPD	O2-C2-C3-C4
29	X	3023	MPD	C2-C3-C4-O4
29	X	3012	MPD	C1-C2-C3-C4
29	X	3012	MPD	O2-C2-C3-C4
29	X	3012	MPD	C2-C3-C4-C5

There are no ring outliers.

25 monomers are involved in 48 short contacts:

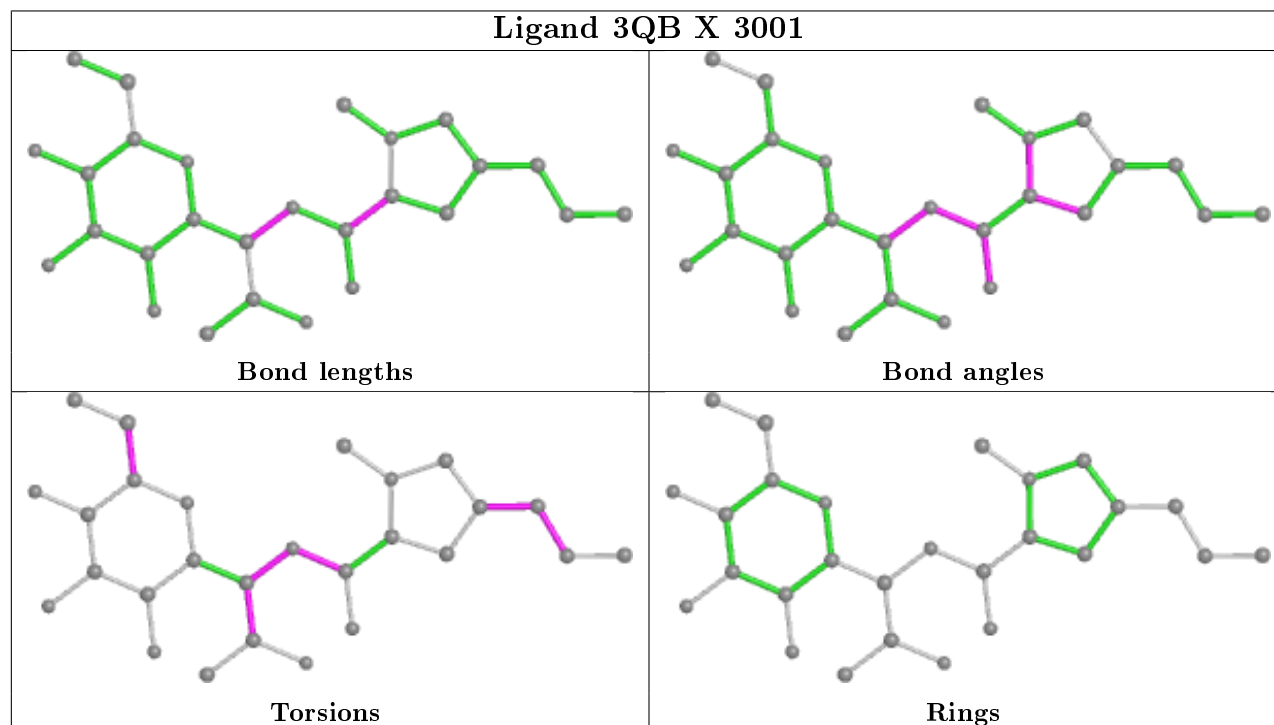
Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	C	303	EOH	2	0
29	X	3012	MPD	1	0
32	X	3489	SPD	10	0
33	R	203	EOH	2	0
29	X	3014	MPD	2	0
29	X	3013	MPD	2	0
32	X	3485	SPD	1	0
29	X	3002	MPD	1	0
29	X	3017	MPD	1	0
33	X	3491	EOH	1	0
29	X	3020	MPD	2	0
32	X	3484	SPD	5	0
32	X	3486	SPD	1	0
29	X	3008	MPD	2	0
29	X	3007	MPD	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	X	3004	MPD	1	0
29	X	3023	MPD	1	0
29	X	3005	MPD	1	0
28	X	3001	3QB	3	0
32	X	3483	SPD	1	0
29	X	3015	MPD	2	0
29	X	3006	MPD	1	0
29	X	3003	MPD	2	0
32	X	3488	SPD	1	0
32	X	3482	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	X	2695/2923 (92%)	-0.40	29 (1%) 80 70	52, 100, 207, 360	0
2	Y	114/114 (100%)	-0.79	0 100 100	68, 128, 188, 250	0
3	A	269/277 (97%)	-0.23	9 (3%) 46 33	73, 131, 198, 239	0
4	B	215/220 (97%)	-0.42	1 (0%) 91 85	59, 78, 120, 186	0
5	C	199/207 (96%)	-0.66	0 100 100	62, 92, 145, 206	0
6	D	166/179 (92%)	0.08	14 (8%) 11 8	120, 196, 267, 336	0
7	E	158/178 (88%)	-0.25	9 (5%) 23 16	99, 178, 251, 279	0
8	G	145/145 (100%)	-0.32	2 (1%) 75 63	56, 74, 107, 170	0
9	H	122/122 (100%)	-0.47	0 100 100	79, 105, 149, 195	0
10	I	131/146 (89%)	-0.29	0 100 100	55, 111, 169, 218	0
11	J	137/144 (95%)	0.54	14 (10%) 6 4	62, 98, 162, 206	0
12	K	119/122 (97%)	0.04	1 (0%) 86 77	59, 87, 139, 234	0
13	L	109/119 (91%)	-0.12	0 100 100	91, 128, 178, 198	0
14	M	108/116 (93%)	-0.24	2 (1%) 66 53	85, 101, 166, 212	0
15	N	116/118 (98%)	-0.13	1 (0%) 84 74	52, 72, 110, 131	0
16	O	102/102 (100%)	-0.17	1 (0%) 82 72	47, 86, 134, 172	0
17	P	112/117 (95%)	0.07	6 (5%) 25 18	63, 74, 129, 191	0
18	Q	89/91 (97%)	-0.18	0 100 100	103, 125, 169, 225	0
19	R	101/105 (96%)	-0.10	3 (2%) 50 36	67, 126, 248, 306	0
20	S	167/217 (76%)	-0.51	1 (0%) 89 83	83, 119, 216, 302	0
21	T	75/94 (79%)	0.24	1 (1%) 77 65	71, 95, 134, 171	0
22	U	42/62 (67%)	3.21	22 (52%) 0 0	148, 193, 238, 279	0
23	V	65/69 (94%)	-0.26	0 100 100	103, 135, 186, 233	0
24	W	57/59 (96%)	-0.23	0 100 100	44, 72, 121, 140	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Z	43/58 (74%)	0.28	3 (6%) 16 10	57, 84, 162, 224	0
26	2	44/45 (97%)	0.08	0 100 100	95, 99, 116, 147	0
27	3	60/66 (90%)	-0.06	0 100 100	58, 84, 115, 153	0
All	All	5760/6215 (92%)	-0.27	119 (2%) 63 50	44, 103, 209, 360	0

The worst 5 of 119 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	U	42	GLY	12.8
22	U	41	ASP	11.9
22	U	47	VAL	9.3
22	U	38	ILE	9.3
22	U	40	VAL	8.3

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
30	MN	X	3087	1/1	0.15	0.88	180,180,180,180	0
30	MN	Y	211	1/1	0.20	0.97	198,198,198,198	0
30	MN	X	3285	1/1	0.38	0.38	163,163,163,163	0
31	MG	L	201	1/1	0.39	0.82	77,77,77,77	0
30	MN	J	201	1/1	0.48	0.22	124,124,124,124	0
30	MN	X	3336	1/1	0.49	0.32	143,143,143,143	0
31	MG	X	3071	1/1	0.51	0.78	87,87,87,87	0
31	MG	X	3106	1/1	0.53	0.61	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
30	MN	X	3197	1/1	0.53	0.19	119,119,119,119	0
30	MN	X	3413	1/1	0.55	0.69	187,187,187,187	0
30	MN	X	3427	1/1	0.55	0.24	161,161,161,161	0
31	MG	X	3078	1/1	0.57	0.31	87,87,87,87	0
30	MN	X	3214	1/1	0.57	0.76	116,116,116,116	0
31	MG	X	3073	1/1	0.61	0.54	98,98,98,98	0
30	MN	X	3430	1/1	0.61	0.61	147,147,147,147	0
30	MN	X	3290	1/1	0.63	0.19	117,117,117,117	0
31	MG	X	3089	1/1	0.63	1.01	89,89,89,89	0
30	MN	X	3387	1/1	0.63	0.17	152,152,152,152	0
31	MG	P	201	1/1	0.64	0.36	120,120,120,120	0
30	MN	X	3431	1/1	0.64	0.86	171,171,171,171	0
30	MN	X	3399	1/1	0.65	0.94	174,174,174,174	0
30	MN	X	3111	1/1	0.65	0.20	178,178,178,178	0
31	MG	X	3077	1/1	0.65	0.50	69,69,69,69	0
30	MN	X	3347	1/1	0.65	0.30	176,176,176,176	0
30	MN	X	3028	1/1	0.66	0.74	226,226,226,226	0
30	MN	X	3195	1/1	0.66	0.36	176,176,176,176	0
30	MN	X	3407	1/1	0.66	0.27	160,160,160,160	0
30	MN	X	3052	1/1	0.67	0.40	154,154,154,154	0
29	MPD	X	3024	8/8	0.67	0.43	159,159,159,159	0
31	MG	P	202	1/1	0.68	0.47	74,74,74,74	0
30	MN	R	202	1/1	0.68	0.11	157,157,157,157	0
30	MN	X	3376	1/1	0.68	0.87	185,185,185,185	0
31	MG	B	301	1/1	0.69	0.53	36,36,36,36	0
30	MN	X	3410	1/1	0.69	0.72	137,137,137,137	0
31	MG	S	302	1/1	0.70	0.41	95,95,95,95	0
31	MG	G	202	1/1	0.70	0.26	70,70,70,70	0
31	MG	X	3074	1/1	0.70	0.58	92,92,92,92	0
30	MN	X	3381	1/1	0.70	0.45	165,165,165,165	0
32	SPD	Y	213	10/10	0.70	0.46	113,113,113,113	0
30	MN	X	3354	1/1	0.71	0.52	127,127,127,127	0
30	MN	X	3188	1/1	0.71	0.18	157,157,157,157	0
30	MN	X	3398	1/1	0.71	0.41	125,125,125,125	0
30	MN	X	3442	1/1	0.71	0.19	141,141,141,141	0
30	MN	X	3382	1/1	0.71	0.58	150,150,150,150	0
30	MN	J	202	1/1	0.71	0.33	137,137,137,137	0
30	MN	X	3189	1/1	0.71	0.34	122,122,122,122	0
30	MN	X	3115	1/1	0.71	0.25	172,172,172,172	0
31	MG	X	3455	1/1	0.71	0.35	73,73,73,73	0
30	MN	X	3178	1/1	0.71	0.44	123,123,123,123	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
30	MN	X	3056	1/1	0.72	0.24	143,143,143,143	0
33	EOH	X	3495	3/3	0.72	0.98	103,103,103,103	0
30	MN	X	3432	1/1	0.72	0.19	133,133,133,133	0
31	MG	X	3450	1/1	0.73	1.03	102,102,102,102	0
30	MN	X	3031	1/1	0.73	0.53	211,211,211,211	0
31	MG	X	3084	1/1	0.73	0.33	80,80,80,80	0
30	MN	X	3117	1/1	0.74	0.52	189,189,189,189	0
31	MG	X	3060	1/1	0.74	0.32	60,60,60,60	0
31	MG	X	3163	1/1	0.74	0.22	90,90,90,90	0
31	MG	X	3108	1/1	0.74	0.47	65,65,65,65	0
31	MG	X	3039	1/1	0.74	0.15	122,122,122,122	0
30	MN	X	3254	1/1	0.74	0.71	183,183,183,183	0
30	MN	A	304	1/1	0.74	0.60	164,164,164,164	0
30	MN	X	3383	1/1	0.75	0.75	172,172,172,172	0
30	MN	X	3288	1/1	0.75	0.51	127,127,127,127	0
30	MN	A	301	1/1	0.75	0.23	184,184,184,184	0
31	MG	X	3103	1/1	0.75	0.48	74,74,74,74	0
30	MN	X	3032	1/1	0.76	1.50	206,206,206,206	0
31	MG	X	3038	1/1	0.76	0.24	100,100,100,100	0
30	MN	X	3348	1/1	0.76	0.12	131,131,131,131	0
30	MN	X	3386	1/1	0.76	0.17	137,137,137,137	0
31	MG	X	3090	1/1	0.76	0.63	87,87,87,87	0
30	MN	Z	101	1/1	0.76	0.56	112,112,112,112	0
30	MN	X	3353	1/1	0.77	0.22	92,92,92,92	0
30	MN	X	3345	1/1	0.77	0.76	140,140,140,140	0
30	MN	X	3242	1/1	0.77	0.25	83,83,83,83	0
31	MG	X	3097	1/1	0.77	0.34	63,63,63,63	0
31	MG	X	3461	1/1	0.77	0.47	104,104,104,104	0
29	MPD	S	301	8/8	0.77	0.30	102,102,102,102	0
30	MN	X	3346	1/1	0.77	1.08	166,166,166,166	0
31	MG	X	3075	1/1	0.78	0.40	88,88,88,88	0
30	MN	X	3358	1/1	0.79	0.65	125,125,125,125	0
30	MN	X	3365	1/1	0.79	0.53	127,127,127,127	0
31	MG	X	3109	1/1	0.79	0.40	82,82,82,82	0
33	EOH	X	3491	3/3	0.79	0.69	85,85,85,85	0
31	MG	X	3063	1/1	0.79	0.21	75,75,75,75	0
31	MG	G	203	1/1	0.80	0.74	74,74,74,74	0
31	MG	X	3058	1/1	0.80	0.30	86,86,86,86	0
30	MN	N	201	1/1	0.80	0.22	166,166,166,166	0
30	MN	X	3393	1/1	0.80	0.08	157,157,157,157	0
30	MN	X	3415	1/1	0.80	0.17	151,151,151,151	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
31	MG	X	3101	1/1	0.80	0.33	85,85,85,85	0
30	MN	X	3343	1/1	0.80	0.51	195,195,195,195	0
30	MN	X	3397	1/1	0.80	0.44	145,145,145,145	0
31	MG	X	3475	1/1	0.80	0.27	80,80,80,80	0
30	MN	X	3394	1/1	0.80	0.09	144,144,144,144	0
31	MG	X	3067	1/1	0.81	0.36	66,66,66,66	0
31	MG	X	3102	1/1	0.81	0.65	72,72,72,72	0
32	SPD	X	3489	10/10	0.81	0.44	96,96,96,96	0
30	MN	X	3267	1/1	0.81	0.51	127,127,127,127	0
30	MN	X	3401	1/1	0.81	0.74	160,160,160,160	0
30	MN	X	3306	1/1	0.81	0.35	122,122,122,122	0
31	MG	K	201	1/1	0.82	0.44	66,66,66,66	0
31	MG	X	3151	1/1	0.82	0.50	61,61,61,61	0
30	MN	X	3206	1/1	0.82	2.08	194,194,194,194	0
29	MPD	X	3022	8/8	0.82	0.39	105,105,105,105	0
31	MG	X	3457	1/1	0.82	0.48	59,59,59,59	0
30	MN	X	3344	1/1	0.82	0.31	143,143,143,143	0
30	MN	C	302	1/1	0.82	0.16	138,138,138,138	0
31	MG	G	201	1/1	0.82	0.16	97,97,97,97	0
30	MN	X	3284	1/1	0.82	0.18	117,117,117,117	0
31	MG	X	3057	1/1	0.82	0.28	73,73,73,73	0
30	MN	X	3400	1/1	0.82	1.09	180,180,180,180	0
30	MN	X	3405	1/1	0.83	0.52	124,124,124,124	0
30	MN	X	3126	1/1	0.83	0.62	158,158,158,158	0
32	SPD	X	3488	10/10	0.83	0.59	79,79,79,79	0
32	SPD	X	3482	10/10	0.83	0.59	135,135,135,135	0
31	MG	X	3081	1/1	0.83	0.21	86,86,86,86	0
30	MN	X	3418	1/1	0.83	0.67	184,184,184,184	0
31	MG	X	3460	1/1	0.83	0.53	82,82,82,82	0
30	MN	X	3338	1/1	0.83	0.13	122,122,122,122	0
31	MG	X	3036	1/1	0.83	0.60	70,70,70,70	0
30	MN	X	3086	1/1	0.83	0.28	211,211,211,211	0
31	MG	X	3045	1/1	0.84	0.18	66,66,66,66	0
30	MN	X	3279	1/1	0.84	0.22	120,120,120,120	0
30	MN	X	3116	1/1	0.84	0.59	190,190,190,190	0
33	EOH	X	3493	3/3	0.84	0.32	100,100,100,100	0
30	MN	Y	201	1/1	0.84	0.50	181,181,181,181	0
30	MN	Y	209	1/1	0.84	0.81	157,157,157,157	0
30	MN	C	301	1/1	0.84	0.10	140,140,140,140	0
32	SPD	X	3487	10/10	0.84	0.31	104,104,104,104	0
31	MG	X	3044	1/1	0.84	0.71	73,73,73,73	0
30	MN	X	3180	1/1	0.84	0.22	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
29	MPD	X	3023	8/8	0.84	0.30	162,162,162,162	0
30	MN	X	3378	1/1	0.84	0.43	173,173,173,173	0
30	MN	X	3373	1/1	0.84	0.41	154,154,154,154	0
30	MN	X	3160	1/1	0.84	0.56	189,189,189,189	0
31	MG	X	3065	1/1	0.85	1.07	88,88,88,88	0
30	MN	X	3426	1/1	0.85	0.28	175,175,175,175	0
30	MN	X	3311	1/1	0.85	0.58	136,136,136,136	0
30	MN	X	3350	1/1	0.85	0.47	168,168,168,168	0
30	MN	X	3292	1/1	0.85	0.70	106,106,106,106	0
31	MG	X	3107	1/1	0.85	0.41	92,92,92,92	0
29	MPD	X	3019	8/8	0.85	0.34	112,112,112,112	0
30	MN	X	3136	1/1	0.85	0.35	103,103,103,103	0
29	MPD	X	3016	8/8	0.85	0.58	114,114,114,114	0
29	MPD	X	3017	8/8	0.85	0.31	135,135,135,135	0
30	MN	X	3224	1/1	0.85	0.65	132,132,132,132	0
31	MG	X	3096	1/1	0.85	0.24	73,73,73,73	0
30	MN	X	3185	1/1	0.85	0.17	95,95,95,95	0
29	MPD	X	3021	8/8	0.85	0.56	130,130,130,130	0
31	MG	X	3162	1/1	0.85	0.58	90,90,90,90	0
30	MN	X	3371	1/1	0.85	0.46	125,125,125,125	0
31	MG	X	3094	1/1	0.86	0.36	63,63,63,63	0
30	MN	X	3198	1/1	0.86	0.18	175,175,175,175	0
30	MN	X	3159	1/1	0.86	1.29	186,186,186,186	0
30	MN	X	3425	1/1	0.86	0.26	129,129,129,129	0
30	MN	X	3423	1/1	0.86	0.14	147,147,147,147	0
30	MN	X	3274	1/1	0.86	0.31	117,117,117,117	0
30	MN	X	3414	1/1	0.86	0.26	146,146,146,146	0
30	MN	X	3417	1/1	0.86	0.34	288,288,288,288	0
31	MG	X	3098	1/1	0.86	0.93	73,73,73,73	0
30	MN	X	3402	1/1	0.86	0.29	156,156,156,156	0
31	MG	X	3037	1/1	0.86	0.38	58,58,58,58	0
30	MN	X	3252	1/1	0.86	0.32	100,100,100,100	0
30	MN	X	3025	1/1	0.86	0.87	222,222,222,222	0
31	MG	X	3105	1/1	0.86	0.46	80,80,80,80	0
30	MN	X	3315	1/1	0.86	0.70	134,134,134,134	0
30	MN	X	3357	1/1	0.86	1.60	172,172,172,172	0
31	MG	X	3148	1/1	0.86	0.39	88,88,88,88	0
31	MG	X	3085	1/1	0.86	0.25	93,93,93,93	0
31	MG	X	3110	1/1	0.86	0.43	87,87,87,87	0
30	MN	X	3175	1/1	0.86	0.21	132,132,132,132	0
31	MG	X	3099	1/1	0.87	0.61	88,88,88,88	0
30	MN	X	3088	1/1	0.87	0.29	151,151,151,151	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
31	MG	X	3041	1/1	0.87	0.86	76,76,76,76	0
31	MG	X	3474	1/1	0.87	0.33	75,75,75,75	0
30	MN	X	3278	1/1	0.87	0.23	144,144,144,144	0
33	EOH	X	3490	3/3	0.87	0.62	65,65,65,65	0
30	MN	X	3128	1/1	0.87	0.35	137,137,137,137	0
32	SPD	X	3483	10/10	0.87	0.26	81,81,81,81	0
30	MN	X	3026	1/1	0.87	0.46	222,222,222,222	0
30	MN	X	3422	1/1	0.88	0.14	134,134,134,134	0
30	MN	X	3250	1/1	0.88	0.28	103,103,103,103	0
31	MG	X	3155	1/1	0.88	0.30	38,38,38,38	0
29	MPD	X	3007	8/8	0.88	0.61	191,191,191,191	0
30	MN	X	3179	1/1	0.88	0.13	121,121,121,121	0
30	MN	X	3030	1/1	0.88	0.39	153,153,153,153	0
31	MG	X	3083	1/1	0.88	0.29	79,79,79,79	0
30	MN	X	3385	1/1	0.88	0.17	153,153,153,153	0
31	MG	X	3079	1/1	0.88	0.14	55,55,55,55	0
30	MN	X	3433	1/1	0.88	0.21	151,151,151,151	0
31	MG	X	3033	1/1	0.88	0.16	77,77,77,77	0
30	MN	X	3396	1/1	0.88	0.46	161,161,161,161	0
30	MN	X	3339	1/1	0.88	0.24	115,115,115,115	0
31	MG	A	302	1/1	0.88	0.23	83,83,83,83	0
31	MG	3	102	1/1	0.88	0.46	55,55,55,55	0
30	MN	X	3029	1/1	0.88	0.14	191,191,191,191	0
29	MPD	X	3009	8/8	0.88	0.56	115,115,115,115	0
31	MG	X	3454	1/1	0.89	0.33	74,74,74,74	0
31	MG	X	3466	1/1	0.89	0.55	77,77,77,77	0
31	MG	X	3476	1/1	0.89	0.44	60,60,60,60	0
31	MG	X	3445	1/1	0.89	0.83	72,72,72,72	0
30	MN	X	3272	1/1	0.89	0.38	114,114,114,114	0
31	MG	X	3048	1/1	0.89	0.21	59,59,59,59	0
31	MG	A	305	1/1	0.89	0.34	72,72,72,72	0
29	MPD	X	3012	8/8	0.89	0.37	116,116,116,116	0
29	MPD	X	3018	8/8	0.89	0.37	141,141,141,141	0
30	MN	X	3404	1/1	0.89	0.13	160,160,160,160	0
30	MN	X	3416	1/1	0.89	0.42	187,187,187,187	0
30	MN	X	3312	1/1	0.89	0.36	97,97,97,97	0
31	MG	A	303	1/1	0.89	0.37	65,65,65,65	0
30	MN	X	3332	1/1	0.89	0.47	144,144,144,144	0
30	MN	X	3127	1/1	0.89	0.48	139,139,139,139	0
30	MN	X	3377	1/1	0.89	0.30	119,119,119,119	0
31	MG	X	3043	1/1	0.89	1.16	82,82,82,82	0
31	MG	X	3149	1/1	0.89	0.20	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
31	MG	X	3456	1/1	0.89	0.78	59,59,59,59	0
30	MN	X	3395	1/1	0.90	0.23	105,105,105,105	0
30	MN	X	3055	1/1	0.90	0.28	195,195,195,195	0
30	MN	X	3437	1/1	0.90	0.39	160,160,160,160	0
30	MN	X	3161	1/1	0.90	0.51	138,138,138,138	0
30	MN	X	3319	1/1	0.90	0.44	115,115,115,115	0
31	MG	X	3059	1/1	0.90	0.17	80,80,80,80	0
31	MG	X	3082	1/1	0.90	0.27	86,86,86,86	0
31	MG	X	3459	1/1	0.90	0.22	44,44,44,44	0
30	MN	Y	210	1/1	0.90	0.23	140,140,140,140	0
30	MN	X	3113	1/1	0.90	0.13	179,179,179,179	0
31	MG	X	3467	1/1	0.90	0.71	68,68,68,68	0
30	MN	X	3218	1/1	0.90	0.47	83,83,83,83	0
30	MN	X	3202	1/1	0.90	0.11	97,97,97,97	0
29	MPD	X	3020	8/8	0.90	0.22	138,138,138,138	0
30	MN	X	3435	1/1	0.90	0.46	67,67,67,67	0
31	MG	X	3070	1/1	0.90	0.26	77,77,77,77	0
30	MN	X	3230	1/1	0.90	0.51	102,102,102,102	0
30	MN	X	3271	1/1	0.90	0.27	100,100,100,100	0
30	MN	X	3428	1/1	0.90	0.13	206,206,206,206	0
32	SPD	X	3486	10/10	0.90	0.61	119,119,119,119	0
30	MN	X	3235	1/1	0.90	0.18	55,55,55,55	0
29	MPD	X	3014	8/8	0.90	0.18	121,121,121,121	0
30	MN	X	3193	1/1	0.90	0.14	119,119,119,119	0
30	MN	X	3424	1/1	0.90	0.14	146,146,146,146	0
30	MN	X	3169	1/1	0.90	1.21	167,167,167,167	0
30	MN	X	3352	1/1	0.90	0.13	97,97,97,97	0
31	MG	X	3451	1/1	0.90	0.23	56,56,56,56	0
30	MN	X	3362	1/1	0.90	0.34	137,137,137,137	0
33	EOH	X	3492	3/3	0.90	0.34	27,27,27,27	0
30	MN	S	303	1/1	0.91	0.57	176,176,176,176	0
30	MN	X	3207	1/1	0.91	0.14	148,148,148,148	0
31	MG	Y	205	1/1	0.91	0.33	117,117,117,117	0
32	SPD	X	3485	10/10	0.91	0.24	86,86,86,86	0
29	MPD	X	3015	8/8	0.91	0.38	111,111,111,111	0
30	MN	X	3248	1/1	0.91	0.51	115,115,115,115	0
31	MG	X	3034	1/1	0.91	0.19	92,92,92,92	0
30	MN	X	3391	1/1	0.91	0.17	174,174,174,174	0
30	MN	X	3238	1/1	0.91	0.47	101,101,101,101	0
31	MG	X	3164	1/1	0.91	0.19	70,70,70,70	0
31	MG	X	3143	1/1	0.91	0.14	80,80,80,80	0
29	MPD	X	3003	8/8	0.91	0.25	127,127,127,127	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
33	EOH	X	3496	3/3	0.91	0.14	60,60,60,60	0
33	EOH	R	203	3/3	0.91	0.21	48,48,48,48	0
30	MN	X	3170	1/1	0.91	0.75	136,136,136,136	0
30	MN	X	3253	1/1	0.91	0.14	137,137,137,137	0
30	MN	X	3367	1/1	0.91	0.22	123,123,123,123	0
30	MN	X	3388	1/1	0.91	0.20	169,169,169,169	0
31	MG	X	3104	1/1	0.91	0.29	97,97,97,97	0
30	MN	X	3379	1/1	0.91	0.17	145,145,145,145	0
30	MN	X	3216	1/1	0.91	0.50	103,103,103,103	0
30	MN	X	3349	1/1	0.91	0.15	119,119,119,119	0
30	MN	X	3236	1/1	0.92	0.22	59,59,59,59	0
31	MG	X	3168	1/1	0.92	0.55	81,81,81,81	0
32	SPD	X	3484	10/10	0.92	0.20	91,91,91,91	0
30	MN	X	3268	1/1	0.92	0.56	117,117,117,117	0
30	MN	X	3498	1/1	0.92	0.41	164,164,164,164	0
30	MN	Y	207	1/1	0.92	0.31	117,117,117,117	0
31	MG	T	101	1/1	0.92	0.24	79,79,79,79	0
31	MG	X	3100	1/1	0.92	0.17	60,60,60,60	0
30	MN	X	3118	1/1	0.92	0.31	210,210,210,210	0
31	MG	X	3171	1/1	0.92	0.22	80,80,80,80	0
30	MN	X	3215	1/1	0.92	0.20	91,91,91,91	0
30	MN	X	3412	1/1	0.92	0.45	113,113,113,113	0
31	MG	X	3080	1/1	0.92	0.17	103,103,103,103	0
30	MN	X	3125	1/1	0.92	0.42	157,157,157,157	0
31	MG	X	3154	1/1	0.92	0.30	54,54,54,54	0
30	MN	X	3419	1/1	0.92	0.24	153,153,153,153	0
30	MN	X	3409	1/1	0.92	0.96	160,160,160,160	0
29	MPD	X	3013	8/8	0.92	0.45	123,123,123,123	0
31	MG	X	3131	1/1	0.92	0.58	90,90,90,90	0
30	MN	X	3384	1/1	0.92	0.70	174,174,174,174	0
31	MG	X	3468	1/1	0.92	0.42	60,60,60,60	0
30	MN	X	3441	1/1	0.93	0.23	203,203,203,203	0
31	MG	X	3448	1/1	0.93	0.18	63,63,63,63	0
30	MN	X	3316	1/1	0.93	0.23	91,91,91,91	0
30	MN	X	3124	1/1	0.93	0.79	165,165,165,165	0
31	MG	M	201	1/1	0.93	0.23	58,58,58,58	0
31	MG	R	201	1/1	0.93	0.14	106,106,106,106	0
30	MN	X	3438	1/1	0.93	0.62	171,171,171,171	0
30	MN	Y	212	1/1	0.93	0.52	183,183,183,183	0
30	MN	X	3203	1/1	0.93	0.12	160,160,160,160	0
30	MN	X	3318	1/1	0.93	0.45	94,94,94,94	0
31	MG	X	3463	1/1	0.93	0.92	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
30	MN	X	3123	1/1	0.93	0.21	195,195,195,195	0
30	MN	X	3112	1/1	0.93	0.76	175,175,175,175	0
30	MN	X	3310	1/1	0.93	0.26	106,106,106,106	0
33	EOH	X	3494	3/3	0.93	0.24	49,49,49,49	0
30	MN	X	3421	1/1	0.93	0.13	131,131,131,131	0
30	MN	X	3210	1/1	0.93	0.43	68,68,68,68	0
30	MN	X	3390	1/1	0.93	0.09	143,143,143,143	0
31	MG	X	3470	1/1	0.93	0.23	86,86,86,86	0
31	MG	X	3449	1/1	0.93	0.09	64,64,64,64	0
30	MN	X	3403	1/1	0.93	0.31	147,147,147,147	0
30	MN	X	3275	1/1	0.93	0.16	109,109,109,109	0
30	MN	X	3184	1/1	0.93	0.24	117,117,117,117	0
30	MN	X	3283	1/1	0.93	0.19	92,92,92,92	0
30	MN	X	3182	1/1	0.93	0.25	127,127,127,127	0
30	MN	X	3301	1/1	0.93	0.08	145,145,145,145	0
31	MG	X	3447	1/1	0.93	0.88	85,85,85,85	0
30	MN	X	3138	1/1	0.93	0.43	138,138,138,138	0
30	MN	X	3444	1/1	0.93	0.07	135,135,135,135	0
30	MN	X	3054	1/1	0.93	0.54	155,155,155,155	0
30	MN	X	3380	1/1	0.93	0.18	111,111,111,111	0
30	MN	X	3237	1/1	0.94	0.36	60,60,60,60	0
30	MN	X	3227	1/1	0.94	0.34	92,92,92,92	0
30	MN	X	3223	1/1	0.94	0.24	87,87,87,87	0
31	MG	X	3069	1/1	0.94	0.14	57,57,57,57	0
30	MN	X	3208	1/1	0.94	0.27	72,72,72,72	0
31	MG	X	3446	1/1	0.94	0.75	71,71,71,71	0
30	MN	X	3289	1/1	0.94	0.19	213,213,213,213	0
30	MN	X	3269	1/1	0.94	0.59	125,125,125,125	0
30	MN	X	3114	1/1	0.94	0.47	185,185,185,185	0
30	MN	X	3190	1/1	0.94	0.38	153,153,153,153	0
30	MN	X	3294	1/1	0.94	0.21	92,92,92,92	0
30	MN	X	3355	1/1	0.94	0.12	149,149,149,149	0
31	MG	X	3133	1/1	0.94	0.45	61,61,61,61	0
30	MN	X	3129	1/1	0.94	0.27	140,140,140,140	0
30	MN	X	3120	1/1	0.94	0.12	133,133,133,133	0
31	MG	X	3062	1/1	0.94	0.21	55,55,55,55	0
30	MN	Y	202	1/1	0.94	0.33	170,170,170,170	0
30	MN	X	3212	1/1	0.94	0.39	131,131,131,131	0
30	MN	X	3199	1/1	0.94	0.12	126,126,126,126	0
31	MG	2	101	1/1	0.94	0.66	57,57,57,57	0
29	MPD	X	3006	8/8	0.94	0.22	119,119,119,119	0
29	MPD	X	3002	8/8	0.94	0.44	141,141,141,141	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
30	MN	X	3497	1/1	0.94	0.13	83,83,83,83	0
31	MG	X	3068	1/1	0.94	0.21	74,74,74,74	0
31	MG	X	3464	1/1	0.94	0.23	67,67,67,67	0
31	MG	3	101	1/1	0.94	0.73	56,56,56,56	0
31	MG	X	3035	1/1	0.94	0.90	89,89,89,89	0
31	MG	X	3465	1/1	0.94	0.06	81,81,81,81	0
30	MN	X	3314	1/1	0.94	0.26	85,85,85,85	0
30	MN	X	3183	1/1	0.94	0.17	107,107,107,107	0
30	MN	X	3192	1/1	0.94	0.37	138,138,138,138	0
31	MG	X	3076	1/1	0.94	0.29	53,53,53,53	0
30	MN	X	3392	1/1	0.95	0.17	135,135,135,135	0
31	MG	X	3150	1/1	0.95	0.17	100,100,100,100	0
30	MN	X	3276	1/1	0.95	0.80	131,131,131,131	0
30	MN	X	3299	1/1	0.95	0.20	96,96,96,96	0
29	MPD	X	3004	8/8	0.95	0.15	111,111,111,111	0
30	MN	X	3194	1/1	0.95	0.14	141,141,141,141	0
30	MN	X	3247	1/1	0.95	0.27	96,96,96,96	0
30	MN	X	3429	1/1	0.95	0.24	147,147,147,147	0
30	MN	X	3360	1/1	0.95	0.11	107,107,107,107	0
31	MG	X	3072	1/1	0.95	0.30	84,84,84,84	0
31	MG	X	3050	1/1	0.95	0.27	83,83,83,83	0
30	MN	X	3205	1/1	0.95	0.66	132,132,132,132	0
31	MG	X	3452	1/1	0.95	0.29	63,63,63,63	0
30	MN	X	3420	1/1	0.95	0.07	106,106,106,106	0
31	MG	X	3478	1/1	0.95	0.23	89,89,89,89	0
31	MG	X	3046	1/1	0.95	0.54	66,66,66,66	0
31	MG	X	3093	1/1	0.95	0.24	53,53,53,53	0
30	MN	X	3408	1/1	0.95	0.40	176,176,176,176	0
31	MG	X	3092	1/1	0.95	0.70	90,90,90,90	0
30	MN	X	3174	1/1	0.95	0.44	113,113,113,113	0
30	MN	X	3280	1/1	0.95	0.23	109,109,109,109	0
30	MN	X	3122	1/1	0.95	0.41	160,160,160,160	0
30	MN	X	3173	1/1	0.95	0.41	105,105,105,105	0
30	MN	X	3295	1/1	0.95	0.18	97,97,97,97	0
31	MG	X	3157	1/1	0.95	0.28	64,64,64,64	0
30	MN	X	3270	1/1	0.95	0.35	86,86,86,86	0
30	MN	X	3374	1/1	0.95	0.20	166,166,166,166	0
30	MN	X	3443	1/1	0.95	0.07	139,139,139,139	0
30	MN	X	3243	1/1	0.95	0.63	99,99,99,99	0
31	MG	X	3472	1/1	0.95	0.09	102,102,102,102	0
31	MG	X	3477	1/1	0.95	0.16	80,80,80,80	0
30	MN	X	3264	1/1	0.95	0.09	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
31	MG	X	3158	1/1	0.95	0.81	68,68,68,68	0
31	MG	X	3042	1/1	0.95	0.12	98,98,98,98	0
29	MPD	X	3008	8/8	0.95	0.29	151,151,151,151	0
31	MG	X	3145	1/1	0.95	0.19	113,113,113,113	0
31	MG	X	3049	1/1	0.95	0.36	87,87,87,87	0
30	MN	X	3200	1/1	0.95	0.13	123,123,123,123	0
30	MN	X	3277	1/1	0.95	0.92	123,123,123,123	0
29	MPD	X	3011	8/8	0.95	0.12	140,140,140,140	0
31	MG	X	3153	1/1	0.96	0.15	131,131,131,131	0
31	MG	X	3166	1/1	0.96	0.48	88,88,88,88	0
30	MN	X	3307	1/1	0.96	0.25	106,106,106,106	0
34	CA	Y	203	1/1	0.96	0.37	139,139,139,139	0
30	MN	X	3217	1/1	0.96	0.45	73,73,73,73	0
30	MN	X	3228	1/1	0.96	0.45	95,95,95,95	0
31	MG	X	3152	1/1	0.96	0.54	107,107,107,107	0
30	MN	X	3053	1/1	0.96	0.23	186,186,186,186	0
30	MN	X	3330	1/1	0.96	0.23	77,77,77,77	0
33	EOH	C	303	3/3	0.96	0.18	74,74,74,74	0
30	MN	X	3309	1/1	0.96	0.50	108,108,108,108	0
30	MN	X	3121	1/1	0.96	0.71	187,187,187,187	0
30	MN	X	3369	1/1	0.96	0.12	108,108,108,108	0
30	MN	X	3359	1/1	0.96	0.37	117,117,117,117	0
31	MG	Y	204	1/1	0.96	0.29	64,64,64,64	0
30	MN	X	3291	1/1	0.96	0.40	122,122,122,122	0
31	MG	X	3142	1/1	0.96	0.31	89,89,89,89	0
30	MN	X	3287	1/1	0.96	0.18	89,89,89,89	0
30	MN	X	3281	1/1	0.96	0.22	100,100,100,100	0
30	MN	X	3221	1/1	0.96	0.18	72,72,72,72	0
29	MPD	X	3010	8/8	0.96	0.14	122,122,122,122	0
31	MG	X	3095	1/1	0.96	0.60	60,60,60,60	0
30	MN	X	3389	1/1	0.96	0.17	165,165,165,165	0
30	MN	X	3204	1/1	0.96	0.13	182,182,182,182	0
31	MG	X	3146	1/1	0.96	0.46	68,68,68,68	0
30	MN	X	3337	1/1	0.96	0.25	69,69,69,69	0
30	MN	X	3211	1/1	0.96	0.46	64,64,64,64	0
30	MN	X	3191	1/1	0.96	0.17	124,124,124,124	0
30	MN	X	3329	1/1	0.96	0.27	82,82,82,82	0
30	MN	X	3240	1/1	0.96	0.32	60,60,60,60	0
30	MN	X	3302	1/1	0.96	0.17	164,164,164,164	0
30	MN	X	3261	1/1	0.97	0.24	67,67,67,67	0
30	MN	X	3181	1/1	0.97	0.38	111,111,111,111	0
30	MN	X	3220	1/1	0.97	0.51	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
31	MG	X	3134	1/1	0.97	0.06	86,86,86,86	0
31	MG	X	3061	1/1	0.97	0.41	37,37,37,37	0
31	MG	X	3066	1/1	0.97	0.59	60,60,60,60	0
30	MN	X	3364	1/1	0.97	0.08	94,94,94,94	0
31	MG	X	3147	1/1	0.97	0.24	71,71,71,71	0
30	MN	X	3225	1/1	0.97	0.26	81,81,81,81	0
30	MN	X	3027	1/1	0.97	0.13	189,189,189,189	0
31	MG	O	201	1/1	0.97	0.47	23,23,23,23	0
31	MG	X	3051	1/1	0.97	0.21	74,74,74,74	0
31	MG	X	3139	1/1	0.97	0.31	36,36,36,36	0
30	MN	X	3333	1/1	0.97	0.94	131,131,131,131	0
30	MN	X	3341	1/1	0.97	0.10	92,92,92,92	0
30	MN	X	3366	1/1	0.97	0.09	104,104,104,104	0
30	MN	X	3176	1/1	0.97	0.28	121,121,121,121	0
30	MN	X	3209	1/1	0.97	0.24	79,79,79,79	0
30	MN	X	3239	1/1	0.97	0.33	49,49,49,49	0
31	MG	X	3091	1/1	0.97	0.13	60,60,60,60	0
30	MN	X	3137	1/1	0.97	0.21	145,145,145,145	0
30	MN	X	3263	1/1	0.97	0.36	98,98,98,98	0
30	MN	X	3255	1/1	0.97	0.37	102,102,102,102	0
30	MN	X	3323	1/1	0.97	0.28	44,44,44,44	0
30	MN	X	3440	1/1	0.97	0.21	150,150,150,150	0
31	MG	X	3156	1/1	0.97	0.34	69,69,69,69	0
30	MN	X	3260	1/1	0.97	0.25	92,92,92,92	0
30	MN	X	3317	1/1	0.97	0.27	69,69,69,69	0
31	MG	X	3479	1/1	0.97	0.20	87,87,87,87	0
30	MN	X	3296	1/1	0.97	0.20	93,93,93,93	0
30	MN	X	3130	1/1	0.97	0.23	145,145,145,145	0
31	MG	X	3469	1/1	0.97	0.14	72,72,72,72	0
31	MG	X	3132	1/1	0.97	0.15	54,54,54,54	0
31	MG	X	3165	1/1	0.97	0.40	81,81,81,81	0
31	MG	X	3141	1/1	0.97	0.58	87,87,87,87	0
31	MG	X	3064	1/1	0.97	1.15	110,110,110,110	0
28	3QB	X	3001	27/27	0.97	0.24	47,47,47,47	0
30	MN	X	3119	1/1	0.97	0.46	182,182,182,182	0
31	MG	X	3473	1/1	0.97	0.20	76,76,76,76	0
30	MN	X	3244	1/1	0.97	0.16	85,85,85,85	0
30	MN	X	3375	1/1	0.97	0.06	141,141,141,141	0
30	MN	X	3304	1/1	0.97	0.21	98,98,98,98	0
30	MN	X	3245	1/1	0.97	0.40	88,88,88,88	0
30	MN	X	3286	1/1	0.97	0.21	80,80,80,80	0
30	MN	I	201	1/1	0.97	0.27	86,86,86,86	0

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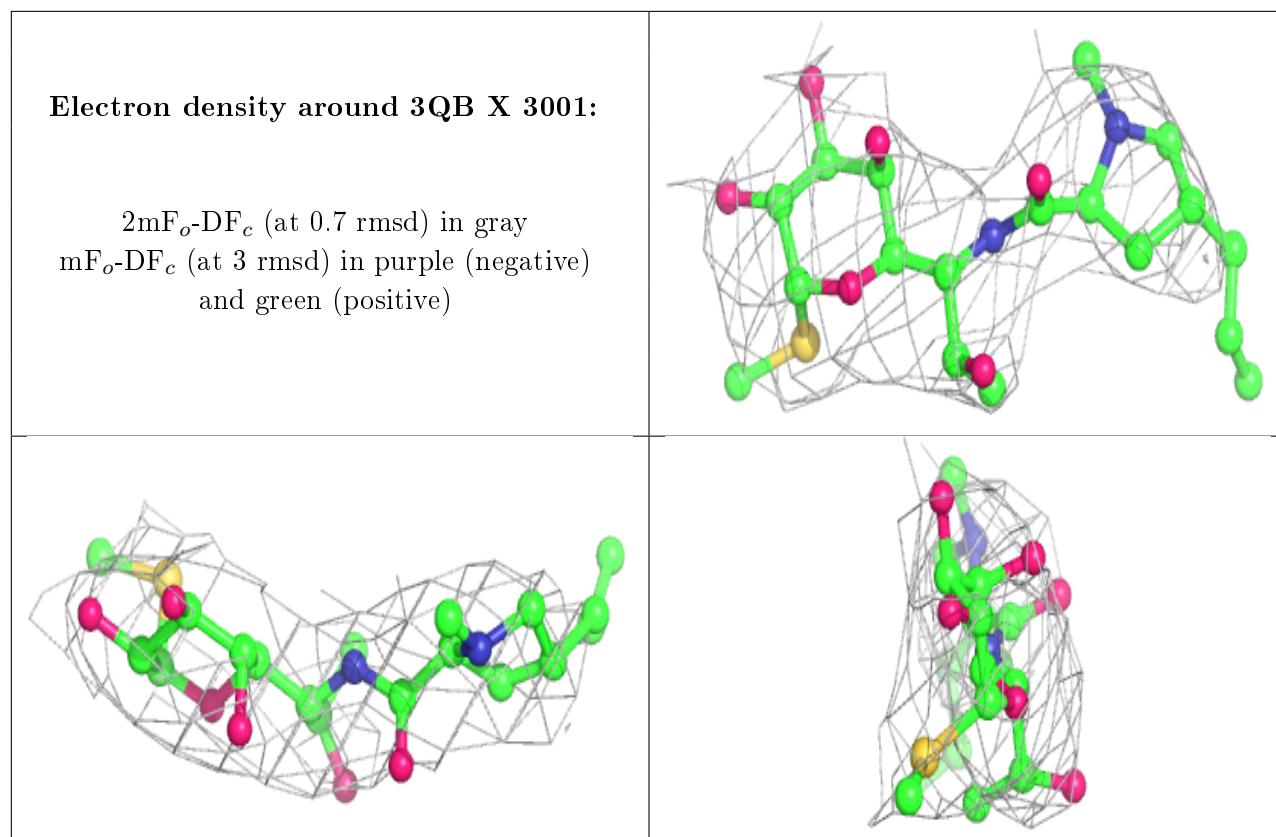
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
29	MPD	X	3005	8/8	0.97	0.36	120,120,120,120	0
30	MN	X	3196	1/1	0.97	0.16	124,124,124,124	0
31	MG	X	3481	1/1	0.98	0.14	60,60,60,60	0
30	MN	X	3436	1/1	0.98	0.24	62,62,62,62	0
31	MG	X	3135	1/1	0.98	0.43	94,94,94,94	0
30	MN	X	3186	1/1	0.98	0.23	111,111,111,111	0
30	MN	X	3372	1/1	0.98	0.07	159,159,159,159	0
30	MN	X	3305	1/1	0.98	0.25	102,102,102,102	0
30	MN	X	3219	1/1	0.98	0.36	68,68,68,68	0
30	MN	X	3368	1/1	0.98	0.16	118,118,118,118	0
31	MG	X	3140	1/1	0.98	0.15	44,44,44,44	0
31	MG	X	3453	1/1	0.98	0.08	92,92,92,92	0
30	MN	X	3406	1/1	0.98	0.15	124,124,124,124	0
30	MN	X	3233	1/1	0.98	0.28	127,127,127,127	0
30	MN	X	3351	1/1	0.98	0.15	99,99,99,99	0
30	MN	X	3273	1/1	0.98	0.19	61,61,61,61	0
30	MN	X	3187	1/1	0.98	0.27	96,96,96,96	0
30	MN	X	3434	1/1	0.98	0.18	96,96,96,96	0
30	MN	X	3177	1/1	0.98	0.25	109,109,109,109	0
30	MN	X	3313	1/1	0.98	0.22	65,65,65,65	0
30	MN	X	3370	1/1	0.98	0.44	153,153,153,153	0
30	MN	X	3266	1/1	0.98	0.21	101,101,101,101	0
30	MN	X	3232	1/1	0.98	0.33	82,82,82,82	0
30	MN	Y	208	1/1	0.98	0.25	107,107,107,107	0
31	MG	Y	206	1/1	0.98	0.21	93,93,93,93	0
31	MG	X	3462	1/1	0.98	0.32	84,84,84,84	0
30	MN	X	3328	1/1	0.98	0.16	93,93,93,93	0
30	MN	X	3300	1/1	0.98	0.32	96,96,96,96	0
30	MN	X	3331	1/1	0.98	0.16	117,117,117,117	0
31	MG	X	3471	1/1	0.98	0.22	101,101,101,101	0
30	MN	X	3257	1/1	0.98	0.12	71,71,71,71	0
30	MN	X	3213	1/1	0.98	0.43	100,100,100,100	0
30	MN	X	3298	1/1	0.98	0.12	129,129,129,129	0
30	MN	X	3201	1/1	0.98	0.08	131,131,131,131	0
30	MN	X	3226	1/1	0.98	0.36	111,111,111,111	0
30	MN	X	3265	1/1	0.98	0.24	60,60,60,60	0
30	MN	X	3326	1/1	0.99	0.27	95,95,95,95	0
30	MN	X	3320	1/1	0.99	0.28	64,64,64,64	0
30	MN	X	3361	1/1	0.99	0.12	89,89,89,89	0
30	MN	X	3172	1/1	0.99	0.19	104,104,104,104	0
30	MN	X	3303	1/1	0.99	0.40	88,88,88,88	0
31	MG	X	3458	1/1	0.99	0.32	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
30	MN	X	3231	1/1	0.99	0.22	87,87,87,87	0
30	MN	X	3308	1/1	0.99	0.14	84,84,84,84	0
31	MG	X	3167	1/1	0.99	0.22	93,93,93,93	0
30	MN	X	3321	1/1	0.99	0.42	78,78,78,78	0
30	MN	X	3356	1/1	0.99	0.17	92,92,92,92	0
30	MN	X	3246	1/1	0.99	0.18	69,69,69,69	0
31	MG	X	3040	1/1	0.99	0.19	111,111,111,111	0
30	MN	X	3249	1/1	0.99	0.17	90,90,90,90	0
30	MN	X	3259	1/1	0.99	0.20	39,39,39,39	0
30	MN	X	3234	1/1	0.99	0.33	61,61,61,61	0
30	MN	X	3327	1/1	0.99	0.18	86,86,86,86	0
30	MN	X	3258	1/1	0.99	0.25	77,77,77,77	0
30	MN	X	3334	1/1	0.99	0.51	112,112,112,112	0
30	MN	X	3439	1/1	0.99	0.46	60,60,60,60	0
30	MN	X	3335	1/1	0.99	0.25	61,61,61,61	0
30	MN	X	3342	1/1	0.99	0.19	85,85,85,85	0
30	MN	X	3297	1/1	0.99	0.13	99,99,99,99	0
30	MN	X	3322	1/1	0.99	0.33	54,54,54,54	0
30	MN	X	3282	1/1	0.99	0.25	80,80,80,80	0
30	MN	X	3222	1/1	0.99	0.24	90,90,90,90	0
30	MN	X	3411	1/1	0.99	0.28	42,42,42,42	0
30	MN	X	3229	1/1	0.99	0.23	93,93,93,93	0
30	MN	X	3363	1/1	0.99	0.21	102,102,102,102	0
31	MG	X	3480	1/1	0.99	0.10	124,124,124,124	0
31	MG	X	3047	1/1	0.99	0.23	35,35,35,35	0
30	MN	X	3262	1/1	0.99	0.36	74,74,74,74	0
30	MN	X	3325	1/1	0.99	0.19	78,78,78,78	0
30	MN	X	3241	1/1	0.99	0.34	49,49,49,49	0
30	MN	X	3324	1/1	0.99	0.17	90,90,90,90	0
30	MN	X	3256	1/1	0.99	0.16	75,75,75,75	0
30	MN	X	3293	1/1	0.99	0.28	84,84,84,84	0
30	MN	X	3251	1/1	0.99	0.15	94,94,94,94	0
30	MN	X	3340	1/1	0.99	0.23	82,82,82,82	0
31	MG	X	3144	1/1	1.00	0.07	75,75,75,75	0

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



6.5 Other polymers [i](#)

There are no such residues in this entry.