



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 22, 2024 – 09:44 AM EDT

PDB ID : 4IOC
Title : Crystal structure of compound 4f bound to large ribosomal subunit (50S) from *Deinococcus radiodurans*
Authors : Han, S.; Marr, E.S.
Deposited on : 2013-01-07
Resolution : 3.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

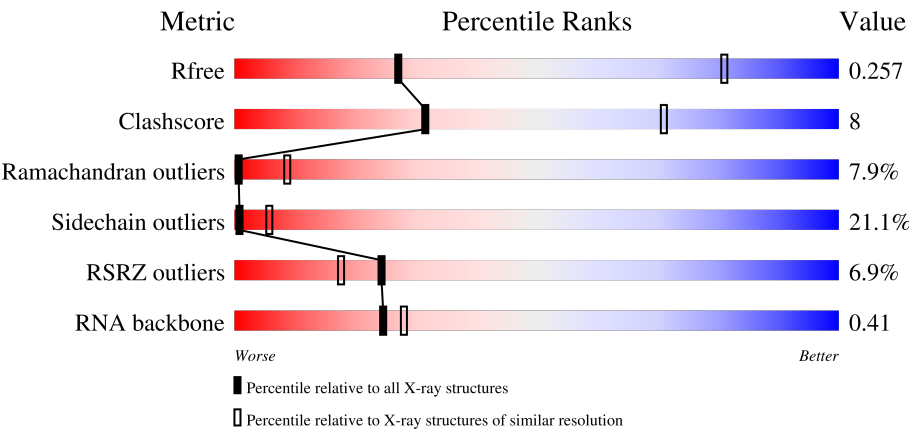
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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}	164625	1563 (3.70-3.50)
Clashscore	180529	1665 (3.70-3.50)
Ramachandran outliers	177936	1641 (3.70-3.50)
Sidechain outliers	177891	1640 (3.70-3.50)
RSRZ outliers	164620	1562 (3.70-3.50)
RNA backbone	3690	1108 (4.20-3.00)

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

Mol	Chain	Length	Quality of chain
1	X	2880	<div><div>3%</div><div><div></div><div></div><div></div><div></div></div><div>30%38%21%•7%</div></div>
2	Y	123	<div><div>2%</div><div><div></div><div></div><div></div><div></div></div><div>27%41%26%6%•</div></div>
3	A	274	<div><div>7%</div><div><div></div><div></div><div></div><div></div></div><div>50%26%11%•12%</div></div>
4	B	211	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>62%26%9%••</div></div>

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Mol	Chain	Length	Quality of chain
5	C	205	
6	D	180	
7	E	185	
8	F	144	
9	G	174	
10	H	134	
11	I	156	
12	J	141	
13	K	116	
14	L	114	
15	M	166	
16	N	118	
17	O	100	
18	P	134	
19	Q	95	
20	R	115	
21	S	237	
22	T	91	
23	U	81	
24	V	67	
25	W	55	
26	Z	60	
27	1	55	
28	2	47	
29	3	66	

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Mol	Chain	Length	Quality of chain
30	4	37	<div> <div>59%</div> <div>70%</div> <div>27%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	MG	M	201	-	-	-	X
31	MG	X	2903	-	-	-	X
31	MG	X	2905	-	-	-	X
31	MG	X	2906	-	-	-	X
31	MG	X	2907	-	-	-	X
31	MG	X	2909	-	-	-	X
31	MG	X	2910	-	-	-	X
31	MG	X	2913	-	-	-	X
31	MG	X	2917	-	-	-	X
31	MG	X	2920	-	-	-	X
31	MG	X	2924	-	-	-	X
31	MG	X	2928	-	-	-	X
31	MG	Y	202	-	-	-	X
31	MG	Y	204	-	-	-	X

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 83877 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	2686	Total	C	N	O	P	0	0	0
			57651	25718	10642	18606	2685			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	122	Total	C	N	O	P	0	0	0
			2598	1161	476	840	121			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	240	Total	C	N	O	S	0	0	0
			1826	1137	366	321	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	205	Total	C	N	O	S	0	0	0
			1539	965	295	271	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	197	Total	C	N	O	S	0	0	0
			1506	935	287	282	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	177	Total	C	N	O	S	0	0	0
			1400	892	247	254	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	171	Total	C	N	O	S	0	0	0
			1286	812	237	236	1			

- Molecule 8 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	71	Total	C	N	O	S	0	0	0
			503	310	91	99	3			

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	G	142	Total	C	N	O	S	0	0	0
			1114	704	209	198	3			

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	H	134	Total	C	N	O	S	0	0	0
			997	614	198	180	5			

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	I	141	Total	C	N	O	0	0	0
			1067	655	216	196			

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	J	136	Total	C	N	O	S	0	0	0
			1090	696	202	185	7			

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	K	113	Total	C	N	O	S	0	0	0
			878	541	178	157	2			

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	L	104	Total	C	N	O	0	0	0
			779	476	161	142			

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	M	108	Total	C	N	O	0	0	0
			871	543	172	156			

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	N	117	Total	C	N	O	S	0	0	0
			978	608	210	159	1			

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	O	94	Total	C	N	O	0	0	0
			741	465	139	137			

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	P	127	Total	C	N	O	S	0	0	0
			1014	639	199	174	2			

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Q	93	Total	C	N	O	S	0	0	0
			726	458	136	130	2			

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	110	Total	C	N	O	S	0	0	0
			825	513	160	151	1			

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	S	175	Total	C	N	O	S	0	0	0
			1345	849	236	254	6			

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	T	84	Total	C	N	O	S	0	0	0
			625	393	122	109	1			

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	U	72	Total	C	N	O		0	0	0
			552	341	116	95				

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	V	66	Total	C	N	O	S	0	0	0
			533	327	107	96	3			

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	W	55	Total	C	N	O	S	0	0	0
			424	264	82	76	2			

- Molecule 26 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	58	Total	C	N	O	S	0	0	0
			457	281	94	77	5			

- Molecule 27 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
27	1	53	Total C	0	0	53
			53 53			

- Molecule 28 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
28	2	46	Total C 46 46	0	0	46

- Molecule 29 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
29	3	63	Total C 63 63	0	0	63

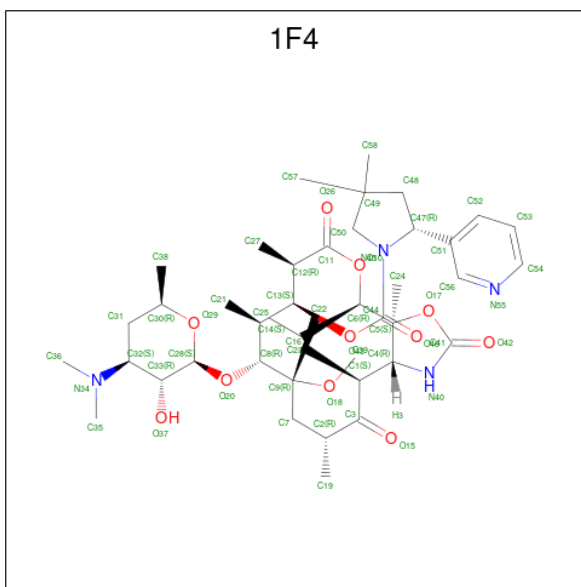
- Molecule 30 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
30	4	37	Total C N O S 297 179 66 47 5	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	X	28	Total Mg 28 28	0	0
31	Y	6	Total Mg 6 6	0	0
31	M	1	Total Mg 1 1	0	0

- Molecule 32 is (3aS,4R,7R,8S,9S,10R,11R,13R,15S,15aR)-4-ethyl-11-methoxy-3a,7,9,11,13,15-hexamethyl-2,6,14-trioxo-10-[[3,4,6-trideoxy-3-(dimethylamino)-beta-D-xylo-hexopyranosyl]oxy]tetradecahydro-2H-oxacyclotetradecino[4,3-d][1,3]oxazol-8-yl (2R)-4,4-dimethyl-2-(pyridin-3-yl)pyrrolidine-1-carboxylate (three-letter code: 1F4) (formula: C₄₃H₆₈N₄O₁₁).

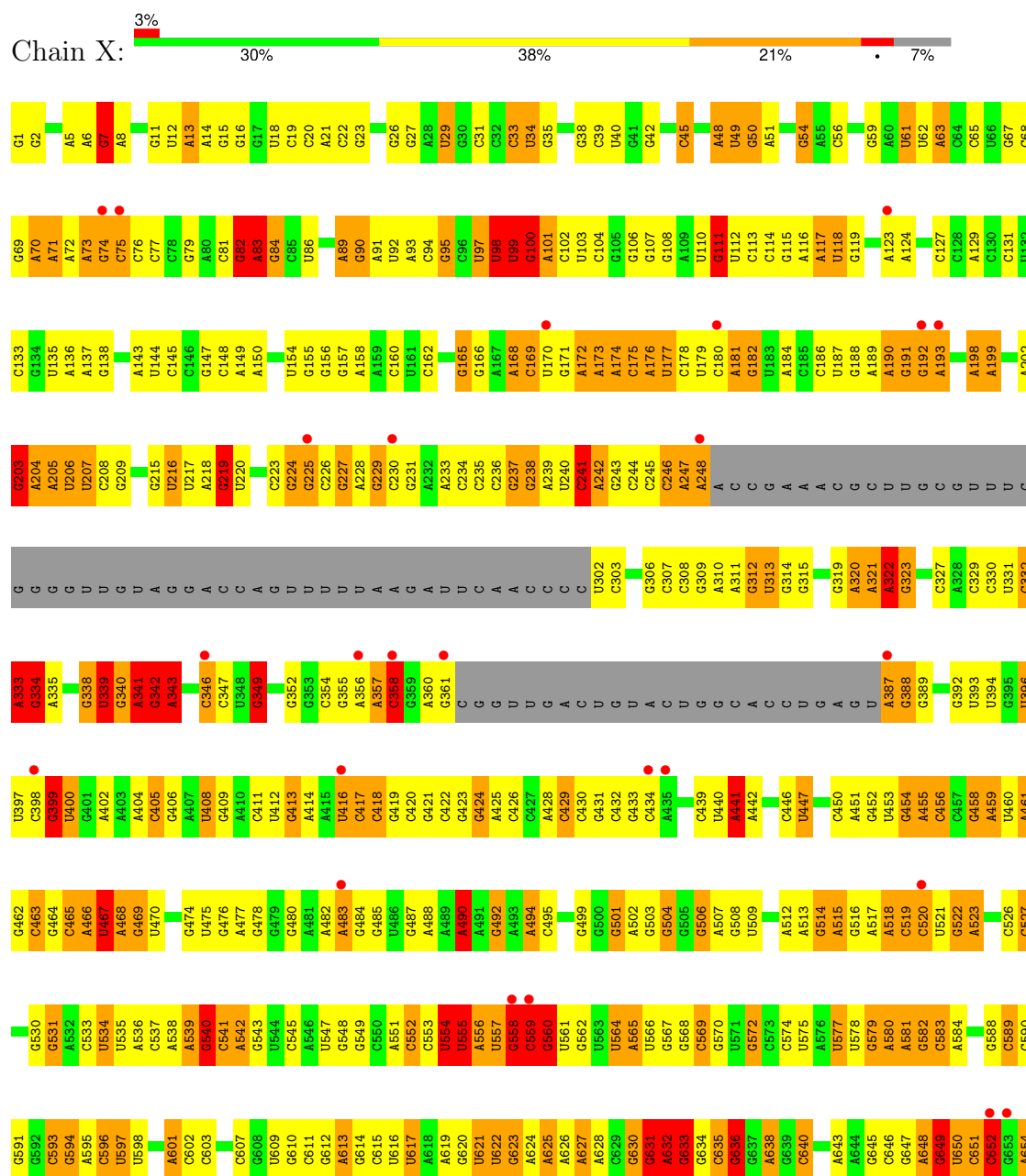


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	X	1	Total	C	N	O	0	0
			58	43	4	11		

3 Residue-property plots

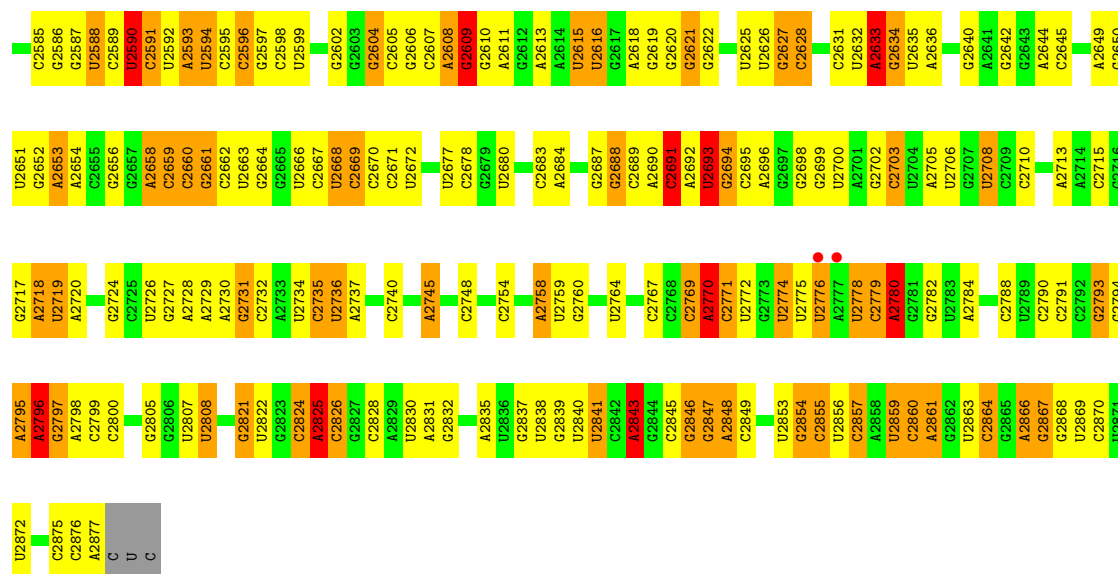
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: 23S ribosomal RNA

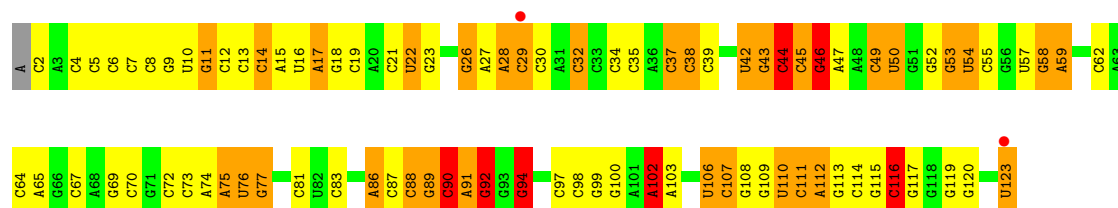




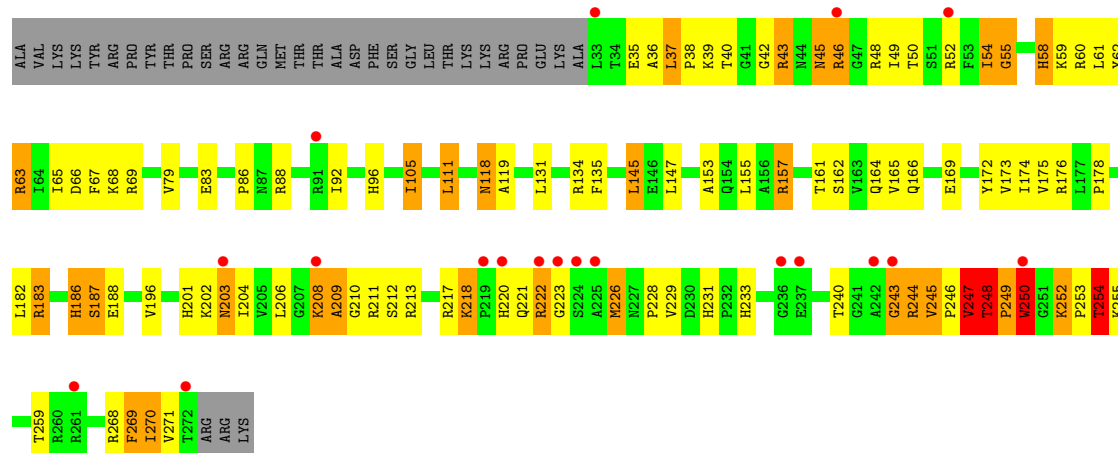




• Molecule 2: 5S ribosomal RNA

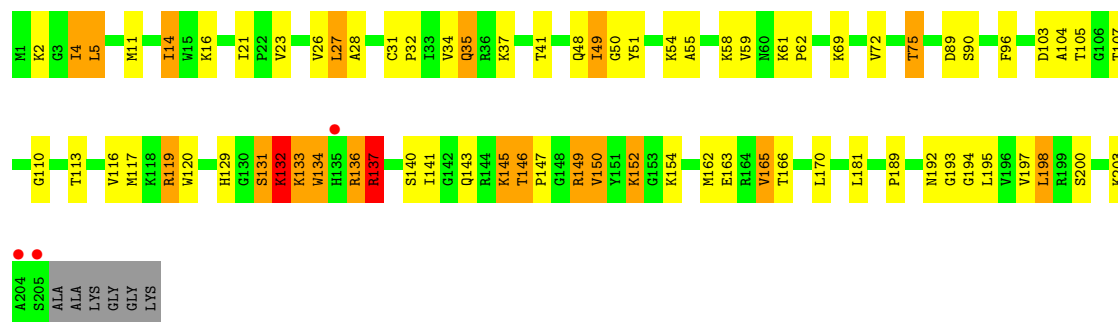


• Molecule 3: 50S ribosomal protein L2

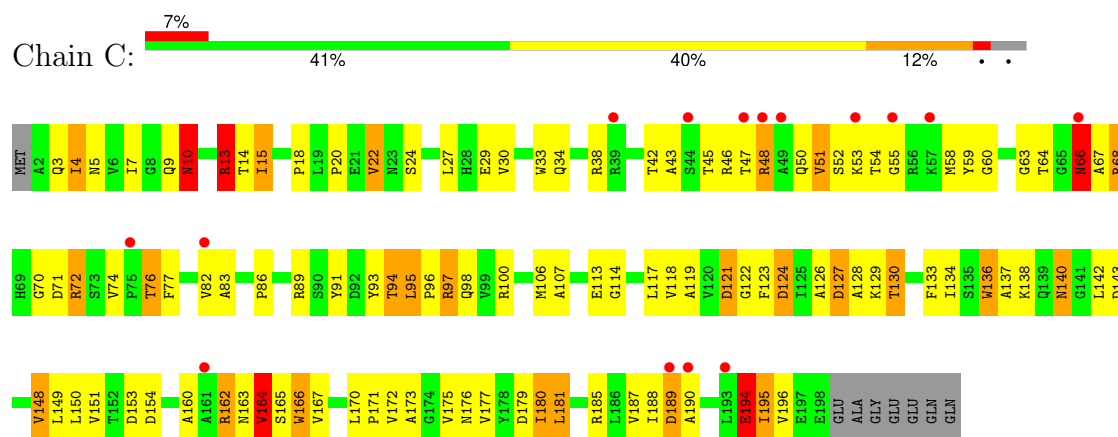


• Molecule 4: 50S ribosomal protein L3

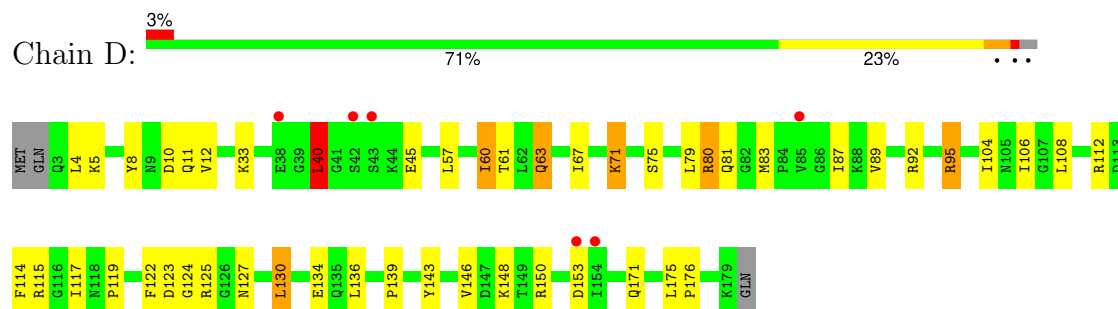




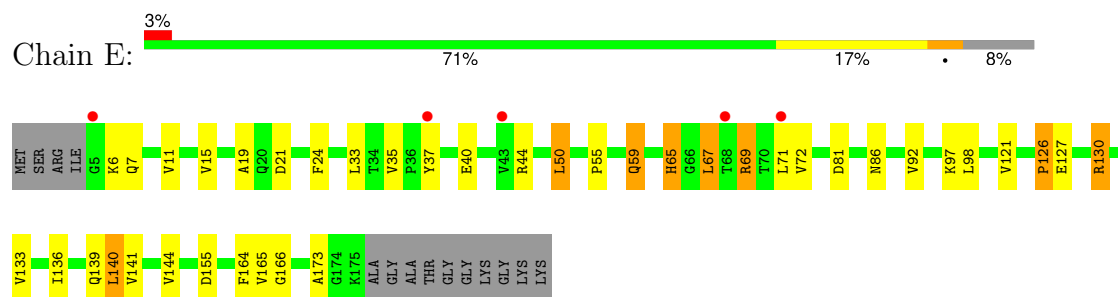
• Molecule 5: 50S ribosomal protein L4



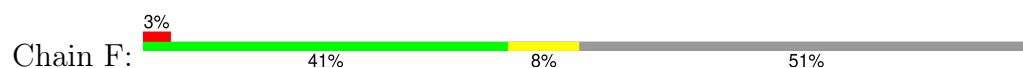
• Molecule 6: 50S ribosomal protein L5

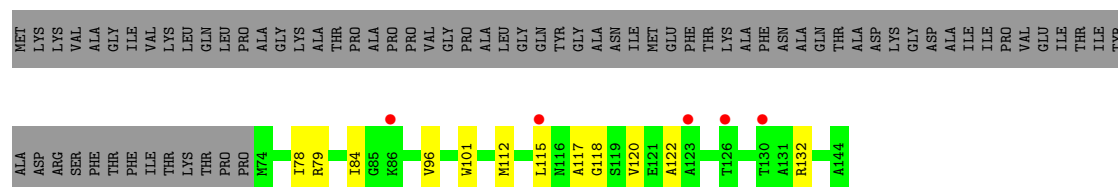


• Molecule 7: 50S ribosomal protein L6

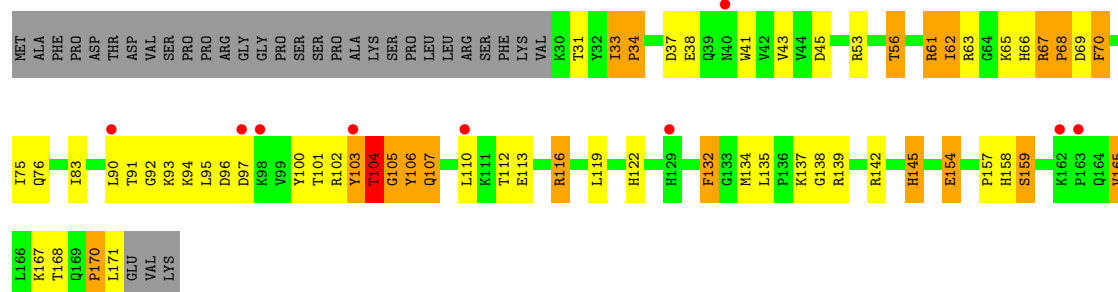


• Molecule 8: 50S ribosomal protein L11

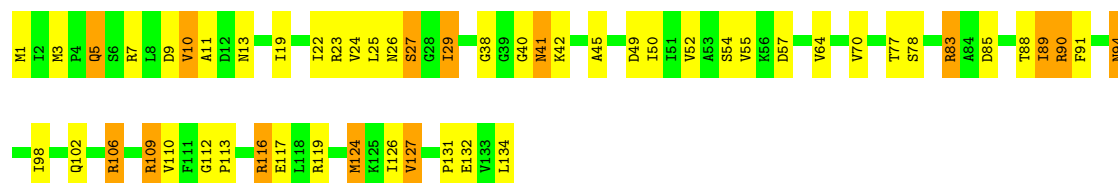




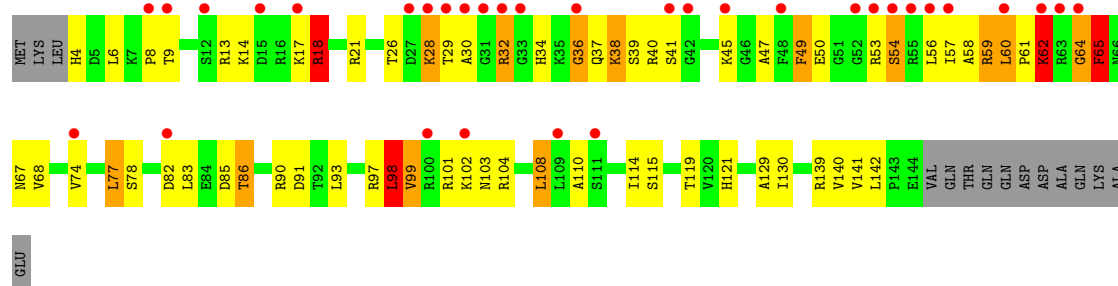
• Molecule 9: 50S ribosomal protein L13



• Molecule 10: 50S ribosomal protein L14



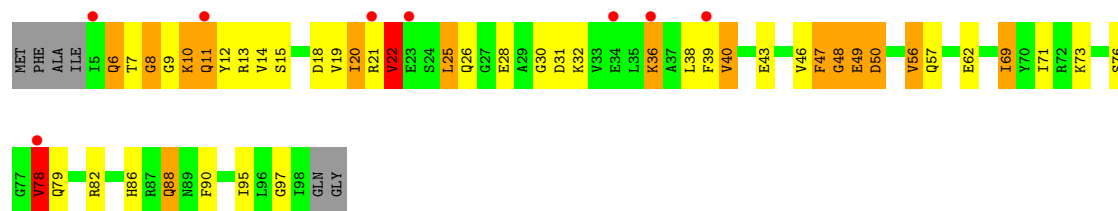
• Molecule 11: 50S ribosomal protein L15



• Molecule 12: 50S ribosomal protein L16

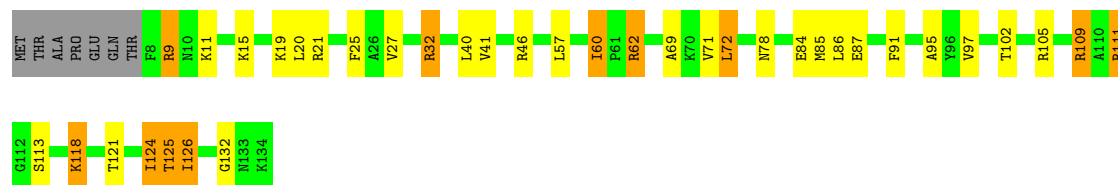






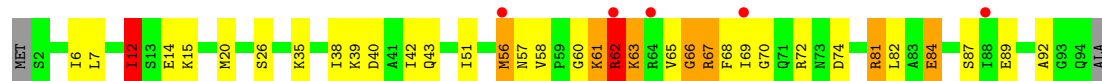
• Molecule 18: 50S ribosomal protein L22

Chain P: 67% 19% 8% 5%



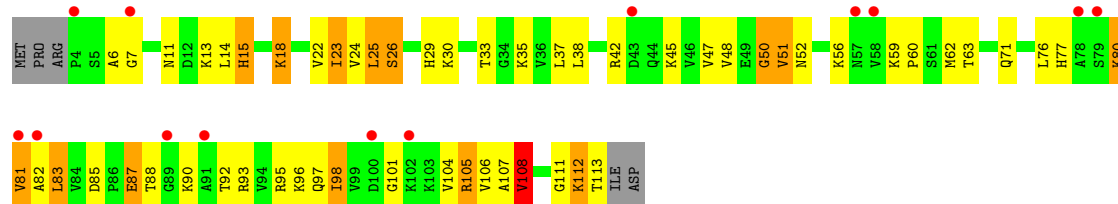
• Molecule 19: 50S ribosomal protein L23

Chain Q: 5% 61% 27% 7%



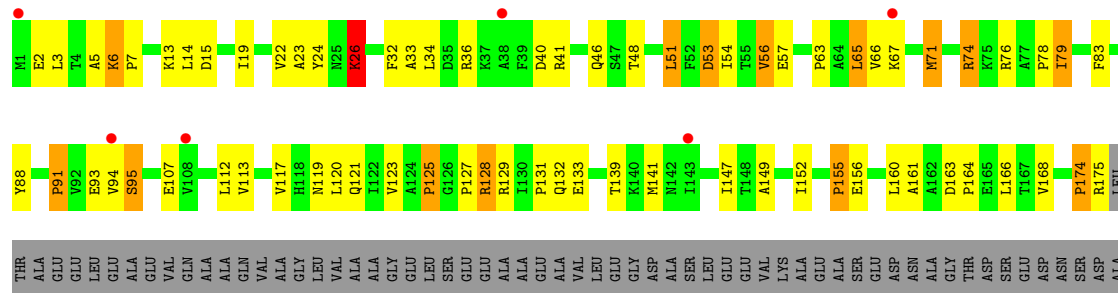
• Molecule 20: 50S ribosomal protein L24

Chain R: 11% 47% 36% 12%



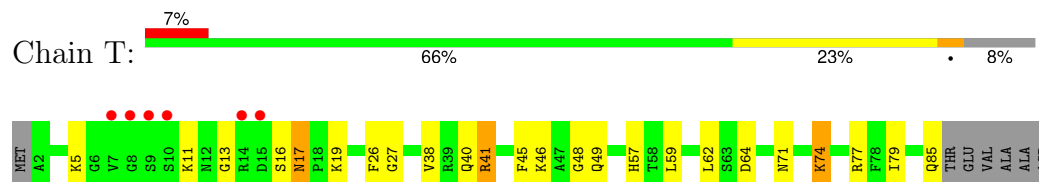
• Molecule 21: 50S ribosomal protein L25

Chain S: 3% 44% 24% 6% 26%

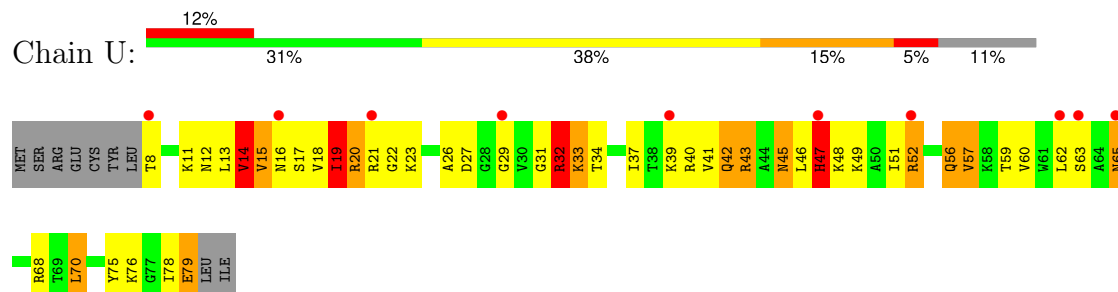


GLN

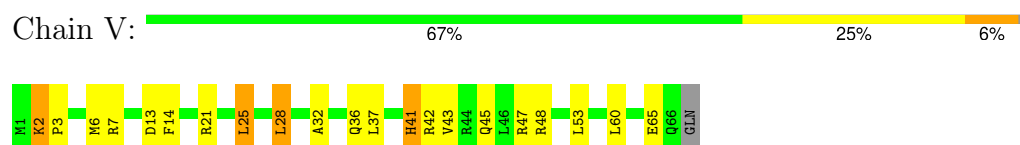
- Molecule 22: 50S ribosomal protein L27



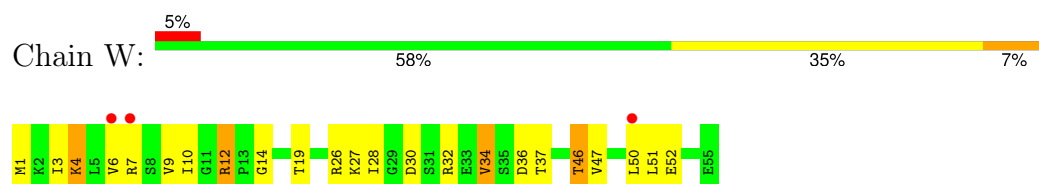
- Molecule 23: 50S ribosomal protein L28



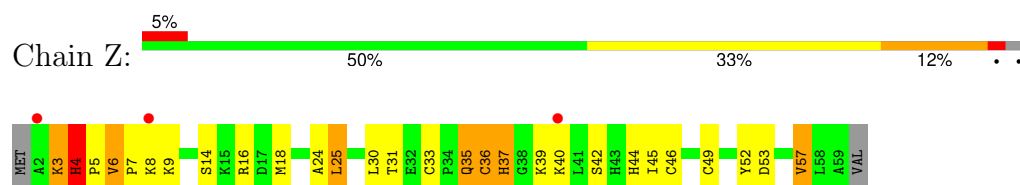
- Molecule 24: 50S ribosomal protein L29



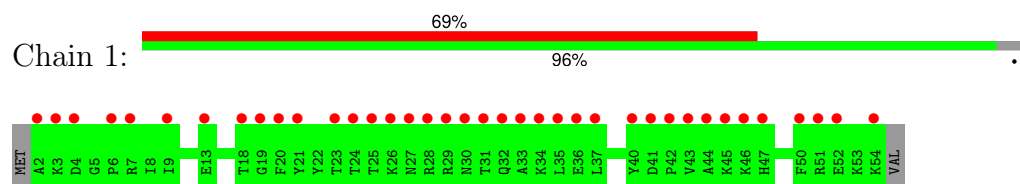
- Molecule 25: 50S ribosomal protein L30



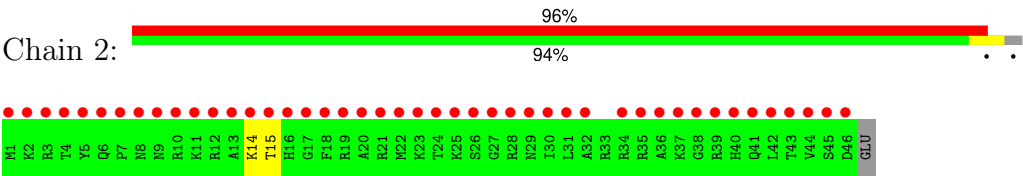
- Molecule 26: 50S ribosomal protein L32



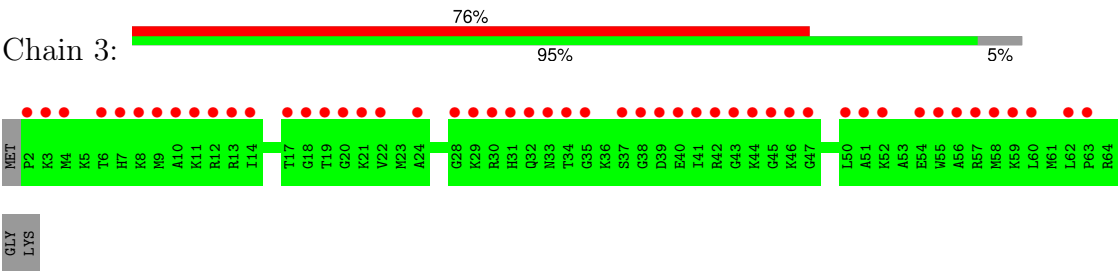
- Molecule 27: 50S ribosomal protein L33



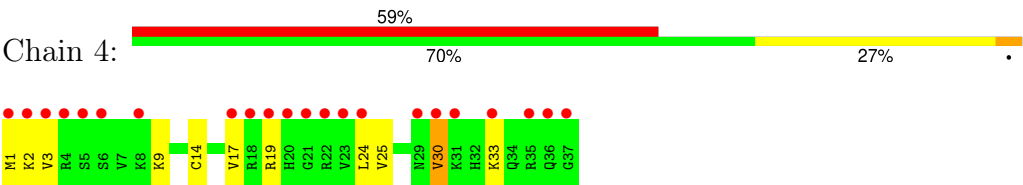
● Molecule 28: 50S ribosomal protein L34



● Molecule 29: 50S ribosomal protein L35



● Molecule 30: 50S ribosomal protein L36



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	169.64Å 408.49Å 692.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.60 30.00 – 3.61	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-3.60) 88.3 (30.00-3.61)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.33 (at 3.65Å)	Xtriage
Refinement program	autoBUSTER	Depositor
R, R_{free}	0.198 , 0.239 0.215 , 0.257	Depositor DCC
R_{free} test set	12232 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	129.2	Xtriage
Anisotropy	0.611	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 91.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	83877	wwPDB-VP
Average B, all atoms (Å ²)	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.08% 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: MG, 1F4

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	1.02	36/64561 (0.1%)	1.86	1991/100708 (2.0%)
2	Y	1.22	2/2904 (0.1%)	1.83	99/4525 (2.2%)
3	A	0.58	0/1862	0.93	4/2510 (0.2%)
4	B	0.55	0/1567	0.88	1/2105 (0.0%)
5	C	0.62	0/1529	0.96	0/2070
6	D	0.46	0/1419	0.68	0/1903
7	E	0.47	0/1308	0.71	0/1771
8	F	0.50	0/508	0.67	0/683
9	G	0.58	0/1138	0.92	2/1539 (0.1%)
10	H	0.53	0/1007	0.84	0/1352
11	I	0.67	0/1081	1.06	2/1448 (0.1%)
12	J	0.86	0/1113	0.96	1/1486 (0.1%)
13	K	0.66	0/886	0.92	0/1188
14	L	0.52	0/785	0.93	0/1048
15	M	0.59	0/884	1.00	2/1186 (0.2%)
16	N	0.53	0/994	0.79	0/1323
17	O	0.52	0/750	0.96	1/1000 (0.1%)
18	P	0.57	0/1027	0.88	0/1373
19	Q	0.56	0/737	0.99	2/988 (0.2%)
20	R	0.59	0/835	1.02	0/1121
21	S	0.61	0/1370	0.76	0/1862
22	T	0.54	0/633	0.88	0/838
23	U	0.71	0/556	1.08	2/741 (0.3%)
24	V	0.52	0/537	0.73	0/714
25	W	0.51	0/426	0.81	0/568
26	Z	0.62	0/469	0.98	0/629
30	4	0.49	0/298	0.73	0/390
All	All	0.94	38/91184 (0.0%)	1.68	2107/137069 (1.5%)

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	X	0	3

The worst 5 of 38 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	559	C	C3'-O3'	8.19	1.53	1.42
1	X	655	A	C3'-O3'	7.84	1.53	1.42
1	X	774	A	C5-C4	7.25	1.43	1.38
1	X	699	G	N9-C4	-6.97	1.32	1.38
1	X	1688	U	C2-N3	6.58	1.42	1.37

The worst 5 of 2107 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1288	A	C1'-O4'-C4'	-30.77	85.29	109.90
1	X	1019	U	P-O3'-C3'	19.01	142.51	119.70
1	X	1288	A	C5'-C4'-O4'	18.79	131.64	109.10
1	X	774	A	N1-C6-N6	17.73	129.24	118.60
1	X	559	C	O4'-C1'-N1	17.43	122.14	108.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	1251	G	Sidechain
1	X	699	G	Sidechain
1	X	967	G	Sidechain

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	57651	0	29049	535	0
2	Y	2598	0	1328	22	0
3	A	1826	0	1885	83	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1539	0	1600	57	0
5	C	1506	0	1525	57	0
6	D	1400	0	1481	17	0
7	E	1286	0	1336	10	0
8	F	503	0	520	5	0
9	G	1114	0	1144	46	0
10	H	997	0	1046	30	0
11	I	1067	0	1103	39	0
12	J	1090	0	1125	31	0
13	K	878	0	930	24	0
14	L	779	0	820	19	0
15	M	871	0	894	25	0
16	N	978	0	1020	33	0
17	O	741	0	756	24	0
18	P	1014	0	1096	23	0
19	Q	726	0	753	11	0
20	R	825	0	881	26	0
21	S	1345	0	1372	30	0
22	T	625	0	655	11	0
23	U	552	0	604	31	0
24	V	533	0	558	7	0
25	W	424	0	470	15	0
26	Z	457	0	462	20	0
27	1	53	0	0	0	0
28	2	46	0	0	1	0
29	3	63	0	0	0	0
30	4	297	0	330	4	0
31	M	1	0	0	0	0
31	X	28	0	0	0	0
31	Y	6	0	0	0	0
32	X	58	0	67	19	0
All	All	83877	0	54810	1080	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 8.

The worst 5 of 1080 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)
4:B:117:MET:SD	4:B:117:MET:CE	2.02	1.47
9:G:100:TYR:HB2	9:G:116:ARG:NH1	1.69	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:33:ILE:HB	9:G:34:PRO:HD3	1.38	1.03
1:X:558:G:H4'	1:X:559:C:H5'	1.40	1.02
1:X:1448:A:H61	1:X:1574:A:H61	1.09	1.00

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	
3	A	238/274 (87%)	173 (73%)	47 (20%)	18 (8%)	1	9
4	B	203/211 (96%)	173 (85%)	25 (12%)	5 (2%)	4	29
5	C	195/205 (95%)	127 (65%)	40 (20%)	28 (14%)	0	3
6	D	175/180 (97%)	142 (81%)	26 (15%)	7 (4%)	2	21
7	E	169/185 (91%)	134 (79%)	26 (15%)	9 (5%)	1	15
8	F	69/144 (48%)	57 (83%)	9 (13%)	3 (4%)	2	19
9	G	140/174 (80%)	99 (71%)	26 (19%)	15 (11%)	0	5
10	H	132/134 (98%)	117 (89%)	12 (9%)	3 (2%)	5	31
11	I	139/156 (89%)	81 (58%)	39 (28%)	19 (14%)	0	3
12	J	134/141 (95%)	98 (73%)	24 (18%)	12 (9%)	0	7
13	K	111/116 (96%)	92 (83%)	13 (12%)	6 (5%)	1	15
14	L	102/114 (90%)	75 (74%)	15 (15%)	12 (12%)	0	4
15	M	106/166 (64%)	90 (85%)	10 (9%)	6 (6%)	1	14
16	N	115/118 (98%)	91 (79%)	17 (15%)	7 (6%)	1	13
17	O	92/100 (92%)	66 (72%)	13 (14%)	13 (14%)	0	3
18	P	125/134 (93%)	104 (83%)	17 (14%)	4 (3%)	3	25
19	Q	91/95 (96%)	63 (69%)	16 (18%)	12 (13%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	R	108/115 (94%)	65 (60%)	26 (24%)	17 (16%)	0	2
21	S	173/237 (73%)	135 (78%)	27 (16%)	11 (6%)	1	13
22	T	82/91 (90%)	65 (79%)	12 (15%)	5 (6%)	1	13
23	U	70/81 (86%)	41 (59%)	15 (21%)	14 (20%)	0	1
24	V	64/67 (96%)	57 (89%)	5 (8%)	2 (3%)	3	26
25	W	53/55 (96%)	47 (89%)	5 (9%)	1 (2%)	6	35
26	Z	56/60 (93%)	45 (80%)	6 (11%)	5 (9%)	0	7
30	4	35/37 (95%)	23 (66%)	11 (31%)	1 (3%)	3	27
All	All	2977/3390 (88%)	2260 (76%)	482 (16%)	235 (8%)	1	9

5 of 235 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	45	ASN
3	A	209	ALA
3	A	217	ARG
3	A	248	THR
3	A	249	PRO

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	185/215 (86%)	145 (78%)	40 (22%)	1	5
4	B	155/157 (99%)	119 (77%)	36 (23%)	0	4
5	C	157/163 (96%)	112 (71%)	45 (29%)	0	2
6	D	153/156 (98%)	130 (85%)	23 (15%)	2	15
7	E	136/144 (94%)	115 (85%)	21 (15%)	2	14
8	F	51/107 (48%)	49 (96%)	2 (4%)	27	57
9	G	118/146 (81%)	94 (80%)	24 (20%)	1	6
10	H	103/103 (100%)	80 (78%)	23 (22%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	I	108/121 (89%)	79 (73%)	29 (27%)	0	2
12	J	110/115 (96%)	89 (81%)	21 (19%)	1	7
13	K	90/93 (97%)	76 (84%)	14 (16%)	2	14
14	L	74/82 (90%)	51 (69%)	23 (31%)	0	2
15	M	94/134 (70%)	71 (76%)	23 (24%)	0	4
16	N	96/97 (99%)	76 (79%)	20 (21%)	1	6
17	O	75/79 (95%)	56 (75%)	19 (25%)	0	3
18	P	109/115 (95%)	91 (84%)	18 (16%)	2	12
19	Q	75/76 (99%)	60 (80%)	15 (20%)	1	6
20	R	91/96 (95%)	75 (82%)	16 (18%)	1	9
21	S	149/192 (78%)	117 (78%)	32 (22%)	1	5
22	T	62/67 (92%)	53 (86%)	9 (14%)	2	16
23	U	57/66 (86%)	33 (58%)	24 (42%)	0	0
24	V	54/55 (98%)	43 (80%)	11 (20%)	1	6
25	W	48/48 (100%)	37 (77%)	11 (23%)	0	4
26	Z	51/53 (96%)	41 (80%)	10 (20%)	1	7
30	4	35/35 (100%)	29 (83%)	6 (17%)	1	10
All	All	2436/2715 (90%)	1921 (79%)	515 (21%)	1	6

5 of 515 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
23	U	40	ARG
23	U	79	GLU
23	U	37	ILE
10	H	10	VAL
9	G	165	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 61 such sidechains are listed below:

Mol	Chain	Res	Type
15	M	90	GLN
23	U	56	GLN
17	O	88	GLN
22	T	71	ASN

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Mol	Chain	Res	Type
26	Z	44	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2683/2880 (93%)	701 (26%)	250 (9%)
2	Y	121/123 (98%)	41 (33%)	12 (9%)
All	All	2804/3003 (93%)	742 (26%)	262 (9%)

5 of 742 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	2	G
1	X	7	G
1	X	13	A
1	X	14	A
1	X	15	G

5 of 262 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	2660	C
1	X	2759	U
2	Y	116	C
1	X	1000	G
1	X	970	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 35 are monoatomic - leaving 1 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	$\# Z > 2$
32	1F4	X	2929	-	61,62,62	1.27	6 (9%)	81,95,95	2.75	37 (45%)

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
32	1F4	X	2929	-	-	33/74/119/119	1/5/5/5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	X	2929	1F4	C41-N40	4.52	1.39	1.33
32	X	2929	1F4	C52-C51	3.41	1.44	1.39
32	X	2929	1F4	C22-C9	2.87	1.58	1.52
32	X	2929	1F4	O46-C44	2.19	1.24	1.21
32	X	2929	1F4	C4-N40	2.09	1.49	1.45

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	X	2929	1F4	C51-C47-N45	-8.29	98.37	113.03
32	X	2929	1F4	C6-O10-C11	6.74	129.97	118.20
32	X	2929	1F4	C22-C9-C7	-5.34	103.00	111.17
32	X	2929	1F4	C21-C14-C13	5.10	120.37	111.40
32	X	2929	1F4	O43-C13-C14	5.05	119.16	107.52

There are no chirality outliers.

5 of 33 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	X	2929	1F4	C4-C5-C6-O10

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Mol	Chain	Res	Type	Atoms
32	X	2929	1F4	C4-C5-C6-C23
32	X	2929	1F4	O17-C5-C6-O10
32	X	2929	1F4	O17-C5-C6-C23
32	X	2929	1F4	C24-C5-C6-O10

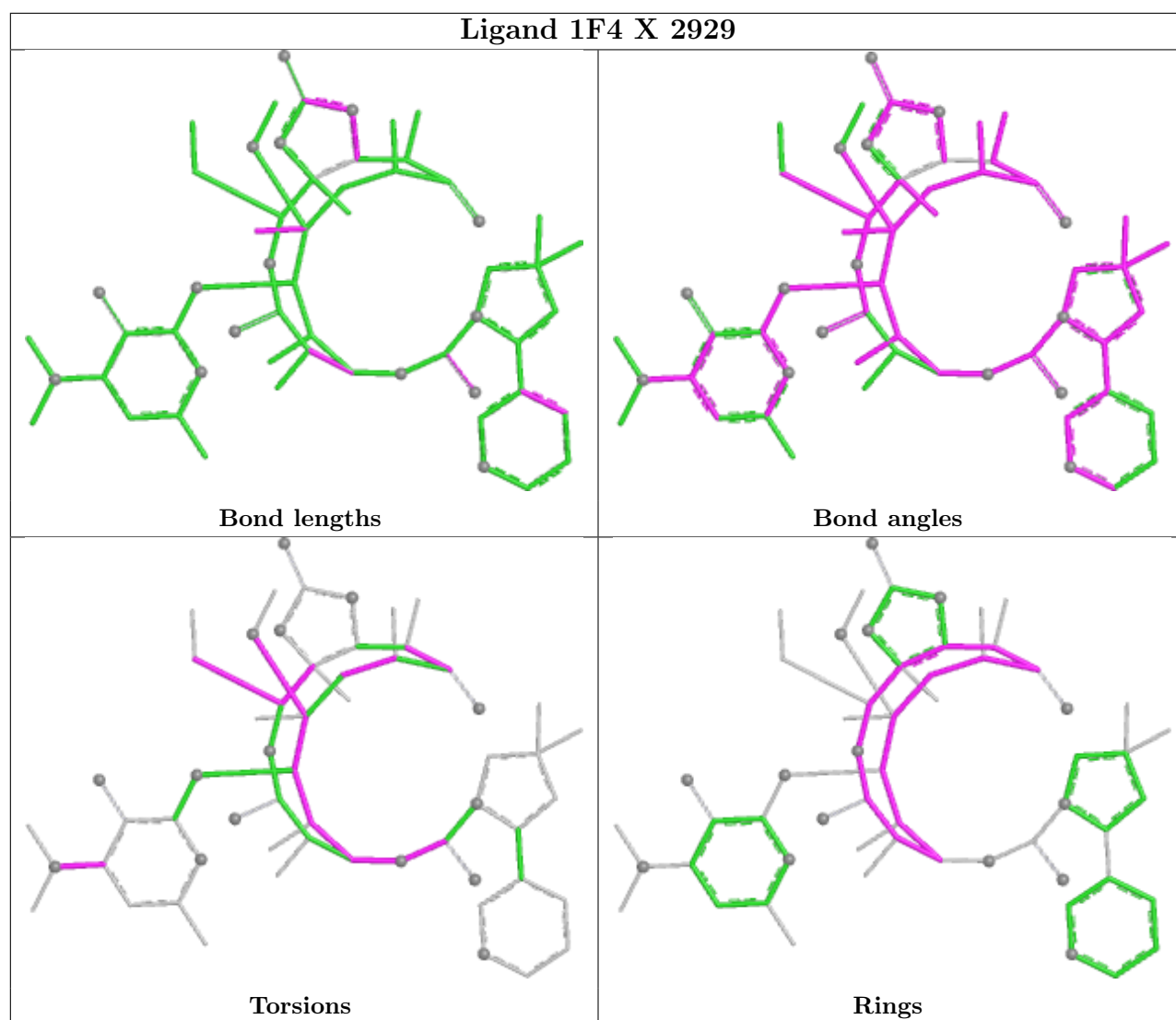
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	X	2929	1F4	C1-C11-C12-C13-C14-C2-C3-C4-C5-C6-C7-C8-C9-O10

1 monomer is involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	X	2929	1F4	19	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	2686/2880 (93%)	-0.07	75 (2%) 55 35	43, 92, 197, 276	0
2	Y	122/123 (99%)	0.13	2 (1%) 70 49	83, 135, 170, 191	0
3	A	240/274 (87%)	0.33	19 (7%) 20 15	68, 115, 146, 172	0
4	B	205/211 (97%)	-0.07	3 (1%) 71 51	45, 73, 105, 154	0
5	C	197/205 (96%)	0.42	15 (7%) 21 16	57, 114, 154, 187	0
6	D	177/180 (98%)	0.18	6 (3%) 48 31	146, 183, 216, 227	0
7	E	171/185 (92%)	-0.06	5 (2%) 54 35	92, 143, 192, 206	0
8	F	71/144 (49%)	0.61	5 (7%) 24 17	211, 236, 252, 257	0
9	G	142/174 (81%)	0.21	9 (6%) 27 19	72, 97, 144, 161	0
10	H	134/134 (100%)	-0.14	0 100 100	50, 70, 97, 121	0
11	I	141/156 (90%)	1.11	33 (23%) 2 3	67, 129, 174, 204	0
12	J	136/141 (96%)	0.26	9 (6%) 26 18	74, 103, 149, 184	0
13	K	113/116 (97%)	0.06	4 (3%) 47 30	35, 60, 79, 91	0
14	L	104/114 (91%)	0.48	12 (11%) 11 9	98, 134, 156, 168	0
15	M	108/166 (65%)	-0.21	0 100 100	50, 73, 111, 145	0
16	N	117/118 (99%)	0.19	8 (6%) 25 18	59, 90, 128, 159	0
17	O	94/100 (94%)	0.22	8 (8%) 18 13	66, 115, 157, 173	0
18	P	127/134 (94%)	-0.32	0 100 100	50, 68, 107, 158	0
19	Q	93/95 (97%)	0.11	5 (5%) 32 22	73, 106, 162, 195	0
20	R	110/115 (95%)	0.51	13 (11%) 10 9	88, 117, 170, 178	0
21	S	175/237 (73%)	0.26	6 (3%) 48 31	121, 155, 175, 190	0
22	T	84/91 (92%)	0.28	6 (7%) 23 17	79, 107, 186, 200	0
23	U	72/81 (88%)	0.81	10 (13%) 7 7	92, 128, 153, 161	0
24	V	66/67 (98%)	-0.41	0 100 100	100, 132, 211, 216	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	W	55/55 (100%)	-0.09	3 (5%) 32 21	80, 98, 126, 152	0
26	Z	58/60 (96%)	0.22	3 (5%) 34 23	49, 70, 105, 114	0
27	1	53/55 (96%)	6.78	38 (71%) 0 0	8, 32, 62, 93	0
28	2	46/47 (97%)	10.33	45 (97%) 0 0	3, 15, 38, 59	0
29	3	63/66 (95%)	8.71	50 (79%) 0 0	3, 25, 40, 61	0
30	4	37/37 (100%)	2.67	22 (59%) 0 0	228, 254, 266, 269	0
All	All	5997/6561 (91%)	0.32	414 (6%) 24 17	3, 100, 196, 276	0

The worst 5 of 414 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
28	2	31	LEU	56.4
27	1	7	ARG	56.0
29	3	28	GLY	43.5
29	3	41	ILE	37.9
27	1	34	LYS	32.1

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 monosaccharides 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.

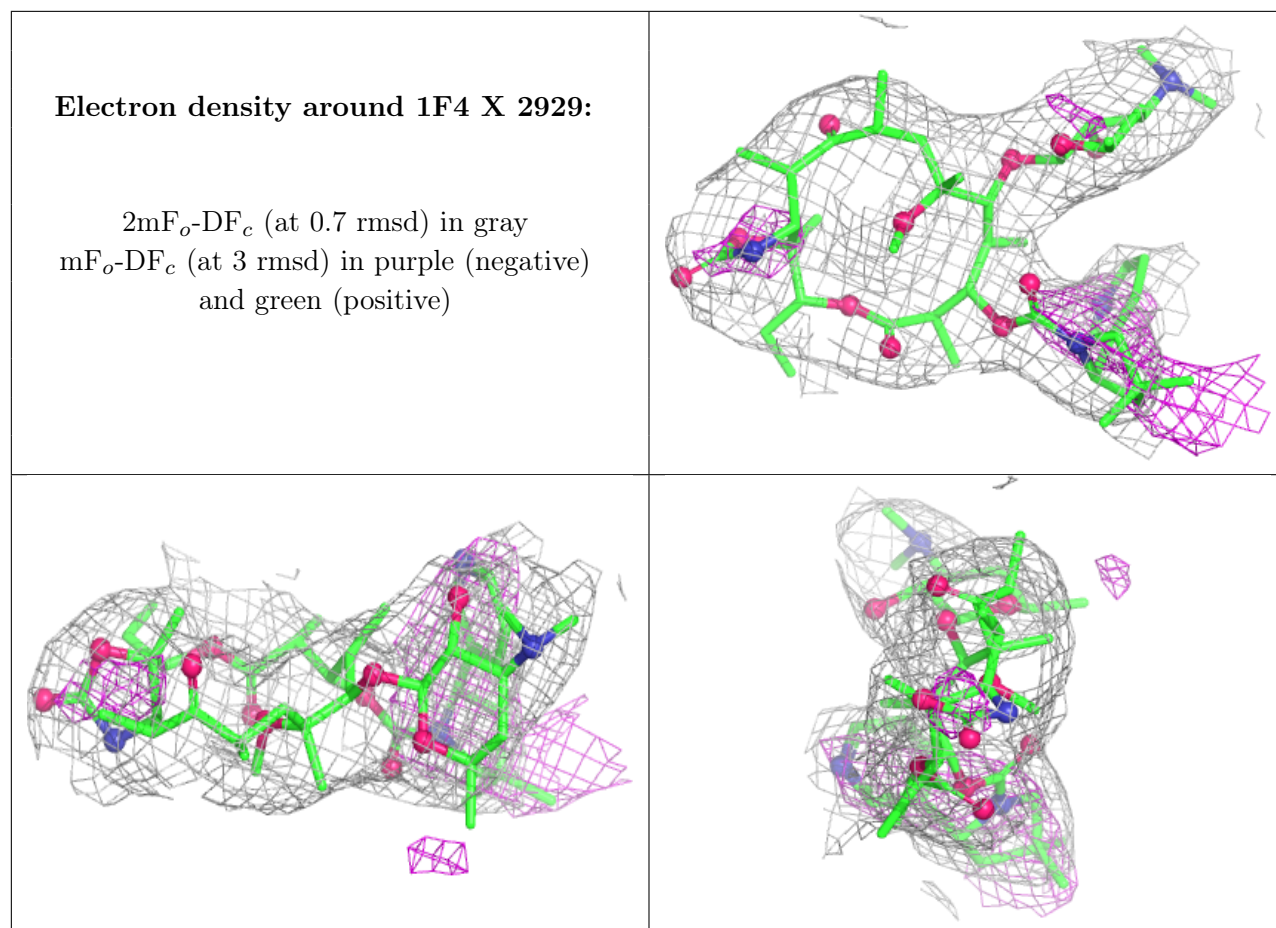
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
31	MG	Y	204	1/1	0.20	0.51	86,86,86,86	0
31	MG	X	2909	1/1	0.25	0.45	97,97,97,97	0
31	MG	Y	202	1/1	0.49	0.92	88,88,88,88	0
31	MG	X	2924	1/1	0.53	0.79	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
31	MG	X	2903	1/1	0.65	1.04	89,89,89,89	0
31	MG	Y	206	1/1	0.67	0.11	78,78,78,78	0
31	MG	X	2913	1/1	0.68	2.54	60,60,60,60	0
31	MG	X	2920	1/1	0.68	0.81	113,113,113,113	0
31	MG	X	2917	1/1	0.70	0.62	55,55,55,55	0
31	MG	X	2928	1/1	0.73	1.28	61,61,61,61	0
31	MG	X	2906	1/1	0.75	0.75	58,58,58,58	0
31	MG	M	201	1/1	0.75	0.47	23,23,23,23	0
31	MG	X	2910	1/1	0.78	0.41	41,41,41,41	0
31	MG	X	2905	1/1	0.78	0.46	65,65,65,65	0
31	MG	X	2907	1/1	0.79	0.77	51,51,51,51	0
31	MG	X	2902	1/1	0.80	0.16	94,94,94,94	0
31	MG	Y	201	1/1	0.80	0.17	98,98,98,98	0
31	MG	X	2914	1/1	0.83	0.40	27,27,27,27	0
31	MG	X	2922	1/1	0.85	0.89	44,44,44,44	0
31	MG	X	2912	1/1	0.85	0.54	71,71,71,71	0
31	MG	X	2925	1/1	0.86	0.20	122,122,122,122	0
31	MG	X	2919	1/1	0.87	0.60	30,30,30,30	0
31	MG	X	2918	1/1	0.88	0.84	42,42,42,42	0
31	MG	X	2915	1/1	0.88	1.64	57,57,57,57	0
31	MG	X	2927	1/1	0.88	0.64	64,64,64,64	0
31	MG	X	2911	1/1	0.89	0.35	68,68,68,68	0
31	MG	X	2921	1/1	0.89	0.82	80,80,80,80	0
31	MG	X	2923	1/1	0.90	0.47	34,34,34,34	0
31	MG	X	2926	1/1	0.90	0.88	45,45,45,45	0
31	MG	X	2908	1/1	0.90	0.73	37,37,37,37	0
31	MG	X	2916	1/1	0.93	0.96	37,37,37,37	0
31	MG	Y	203	1/1	0.94	0.41	59,59,59,59	0
32	1F4	X	2929	58/58	0.94	0.09	20,20,20,20	0
31	MG	Y	205	1/1	0.96	0.19	82,82,82,82	0
31	MG	X	2901	1/1	0.97	1.85	50,50,50,50	0
31	MG	X	2904	1/1	0.97	0.11	110,110,110,110	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.