wwPDB X-ray Structure Validation Summary Report (i)

Jun 18, 2024 – 10:43 AM EDT

PDB ID	:	4B3M
Title	:	Crystal structure of the 30S ribosome in complex with compound 1
Authors	:	Ng, C.L.; Lang, K.; Shcherbakov, D.; Matt, T.; Perez-Fernandez, D.; Patak, R.; Meyer, M.; Duscha, S.; Akbergenov, R.; Boukari, H.; Freihofer, P.; Kudyba, I.; Reddy, M.S.K.; Nandurikar, R.S.; Ramakrishnan, V.; Vasella, A.; Bottger, E.C.
Deposited on	:	2012-07-25
Resolution	:	2.90 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

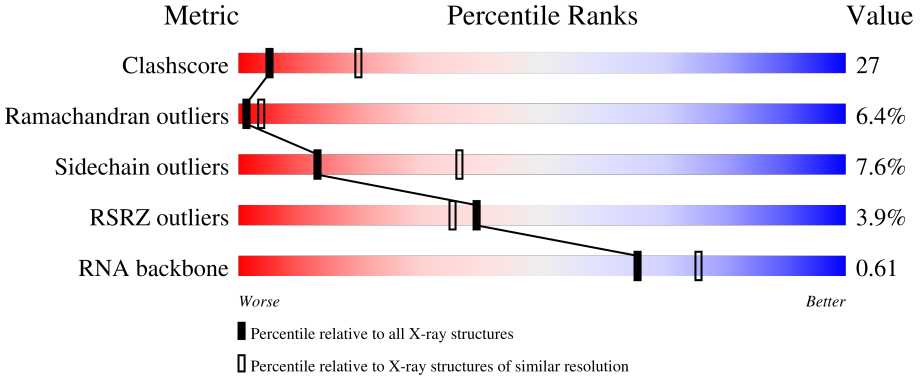
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.90 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))
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)
RNA backbone	3102	1007 (3.16-2.64)

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

Mol	Chain	Length	Quality of chain
1	A	1521	2%, 41%, 45%, 12%
2	B	256	8%, 24%, 53%, 12%, 8%
3	C	239	2%, 32%, 41%, 13%, 13%
4	D	208	5%, 53%, 38%, 8%
5	E	161	45%, 42%, 6%, 6%

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Mol	Chain	Length	Quality of chain
6	F	101	2%, 51%, 48%
7	G	155	4%, 46%, 49%
8	H	138	%, 51%, 42%, 6%
9	I	128	4%, 33%, 59%, 6%
10	J	104	23%, 26%, 54%, 15%, 5%
11	K	129	3%, 41%, 49%, 8%
12	L	132	4%, 52%, 36%, 7%, 5%
13	M	126	12%, 30%, 56%, 12%
14	N	60	7%, 27%, 53%, 18%
15	O	88	2%, 49%, 47%, 5%
16	P	88	52%, 38%, 6%, 5%
17	Q	104	5%, 63%, 28%, 8%
18	R	88	3%, 32%, 45%, 6%, 17%
19	S	92	7%, 27%, 52%, 9%, 12%
20	T	106	5%, 55%, 27%, 11%, 7%
21	V	26	12%, 54%, 42%
22	W	6	33%, 17%, 83%
23	Z	16	6%, 56%, 31%, 12%

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
24	MG	A	2275	-	-	-	X
24	MG	A	2546	-	-	-	X
24	MG	A	2547	-	-	-	X
24	MG	A	2553	-	-	-	X
24	MG	A	2554	-	-	-	X
24	MG	A	2555	-	-	-	X
24	MG	A	2566	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	MG	A	2575	-	-	-	X
24	MG	A	2599	-	-	-	X
24	MG	A	2607	-	-	-	X
24	MG	A	2613	-	-	-	X
24	MG	A	2617	-	-	-	X
24	MG	A	2660	-	-	-	X
24	MG	A	2661	-	-	-	X
24	MG	A	2662	-	-	-	X
24	MG	A	2666	-	-	-	X
24	MG	A	2703	-	-	-	X
24	MG	A	2714	-	-	-	X
24	MG	A	2715	-	-	-	X
24	MG	A	2717	-	-	-	X
24	MG	A	2718	-	-	-	X
24	MG	A	2719	-	-	-	X
24	MG	A	2722	-	-	-	X
24	MG	A	2724	-	-	-	X
24	MG	A	2729	-	-	-	X
24	MG	A	2737	-	-	-	X
24	MG	A	2743	-	-	-	X
24	MG	A	2744	-	-	-	X
24	MG	A	2750	-	-	-	X
24	MG	A	2754	-	-	-	X
24	MG	A	2758	-	-	-	X
24	MG	H	1140	-	-	-	X
24	MG	Z	1043	-	-	-	X
25	K	A	2673	-	-	-	X
25	K	A	2773	-	-	-	X

2 Entry composition (i)

There are 28 unique types of molecules in this entry. The entry contains 52505 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 16S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	1512	32486	14462	6011	10503	1510	0	0	0

- Molecule 2 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	235	1901	1213	342	341	5	0	0	1

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	207	1613	1016	315	281	1	0	0	1

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	208	1703	1066	339	291	7	0	0	0

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	151	1147	724	218	201	4	0	0	1

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	101	843	531	155	154	3	0	0	0

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	G	155	1257	781	252	218	6	0	0	0

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	H	138	1116	705	215	193	3	0	0	0

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
9	I	127	1011	639	198	174	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	57	ARG	HIS	conflict	UNP P80374

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	J	99	795	499	157	138	1	0	0	1

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	K	119	885	549	168	165	3	0	0	0

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	L	125	971	611	196	163	1	0	0	1

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	M	125	997	617	207	171	2	0	0	0

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S14 TYPE Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	N	60	492	312	104	72	4	0	0	0

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	O	88	734	459	147	126	2	0	0	0

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	P	84	701	443	140	117	1	0	0	1

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
17	Q	104	857	547	161	147	2	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	95	GLN	GLU	conflict	UNP Q5SHP7

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
18	R	73	597	380	118	99	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	45	GLY	ALA	conflict	UNP Q5SLQ0

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
19	S	81	648	414	120	112	2	0	0	1

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
20	T	99	762	469	162	129	2	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	34	VAL	ILE	conflict	UNP P80380

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
21	V	25	209	128	51	30	0	0	1

- Molecule 22 is a RNA chain called 5'-R(*UP*UP*CP*AP*AP*AP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
22	W	6	123	57	22	39	5	0	0	0

- Molecule 23 is a RNA chain called 5'-R(*GP*GP*GP*AP*UP*UP*GP*AP*AP*AP*AP*UP*CP*CP*CP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
23	Z	16	342	154	65	108	15	0	0	0

- Molecule 24 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
24	A	223	223	223	0	0
24	B	1	1	1	0	0

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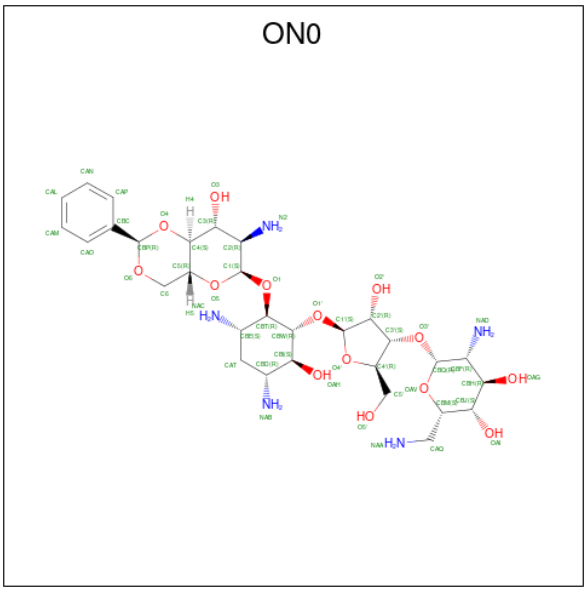
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	D	1	Total Mg 1 1	0	0
24	E	3	Total Mg 3 3	0	0
24	H	4	Total Mg 4 4	0	0
24	I	1	Total Mg 1 1	0	0
24	K	1	Total Mg 1 1	0	0
24	L	1	Total Mg 1 1	0	0
24	M	1	Total Mg 1 1	0	0
24	N	1	Total Mg 1 1	0	0
24	Q	1	Total Mg 1 1	0	0
24	T	1	Total Mg 1 1	0	0
24	Z	1	Total Mg 1 1	0	0

- Molecule 25 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	17	Total K 17 17	0	0

- Molecule 26 is (1R,2R,3S,4R,6S)-4,6-diamino-2-{[3-O-(2,6-diamino-2,6-dideoxy-beta-L-idopyranosyl)-beta-D-ribofuranosyl]oxy}-3-hydroxycyclohexyl 2-amino-4,6-O-benzylidene-2-deoxy-alpha-D-glucopyranoside (three-letter code: ON0) (formula: $C_{30}H_{49}N_5O_{14}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
26	A	1	49	30	5	14	0	0

- Molecule 27 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
27	D	1	1	1	0	0
27	N	1	1	1	0	0

- Molecule 28 is water.

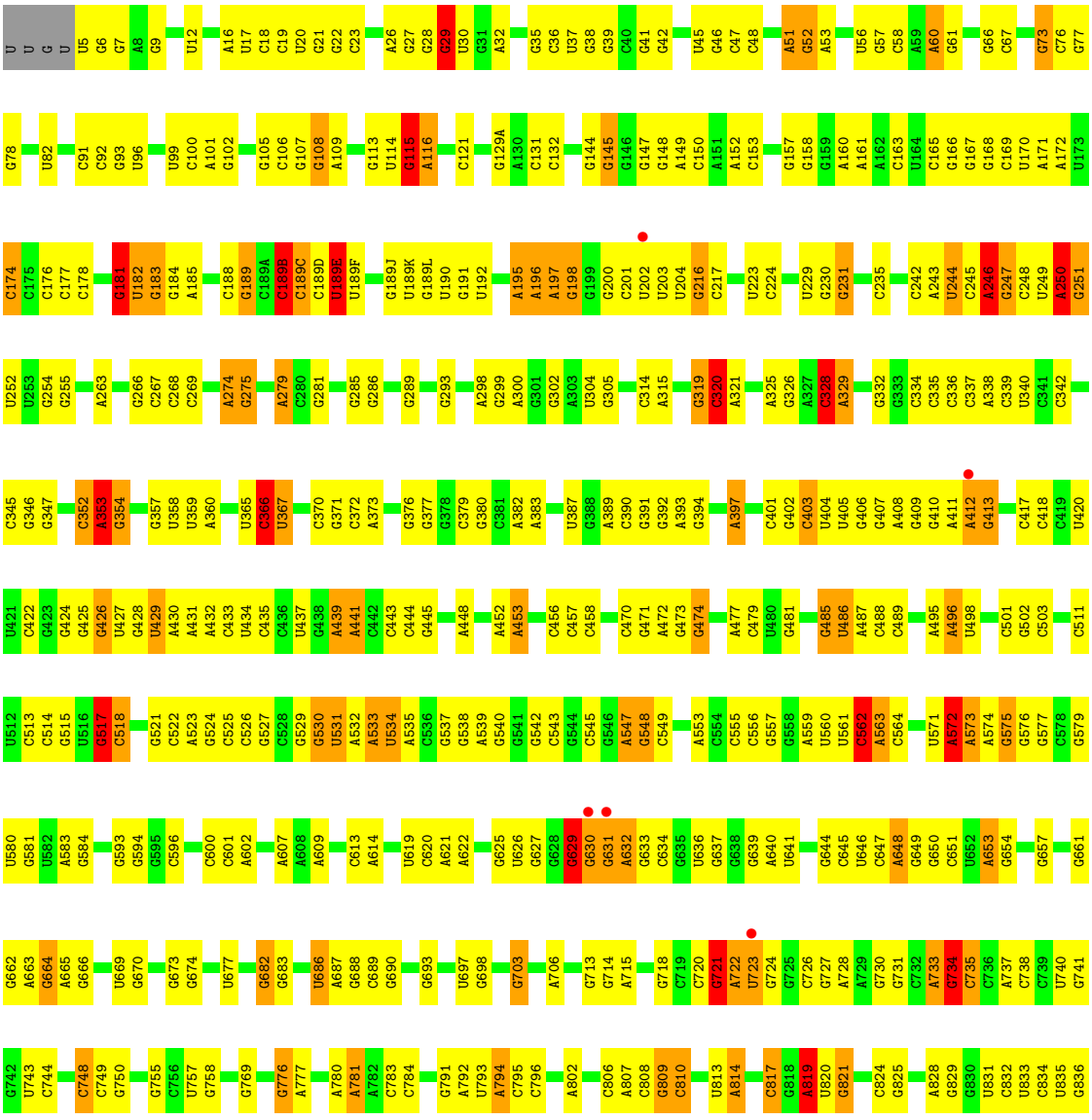
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
28	A	7	7	7	0	0

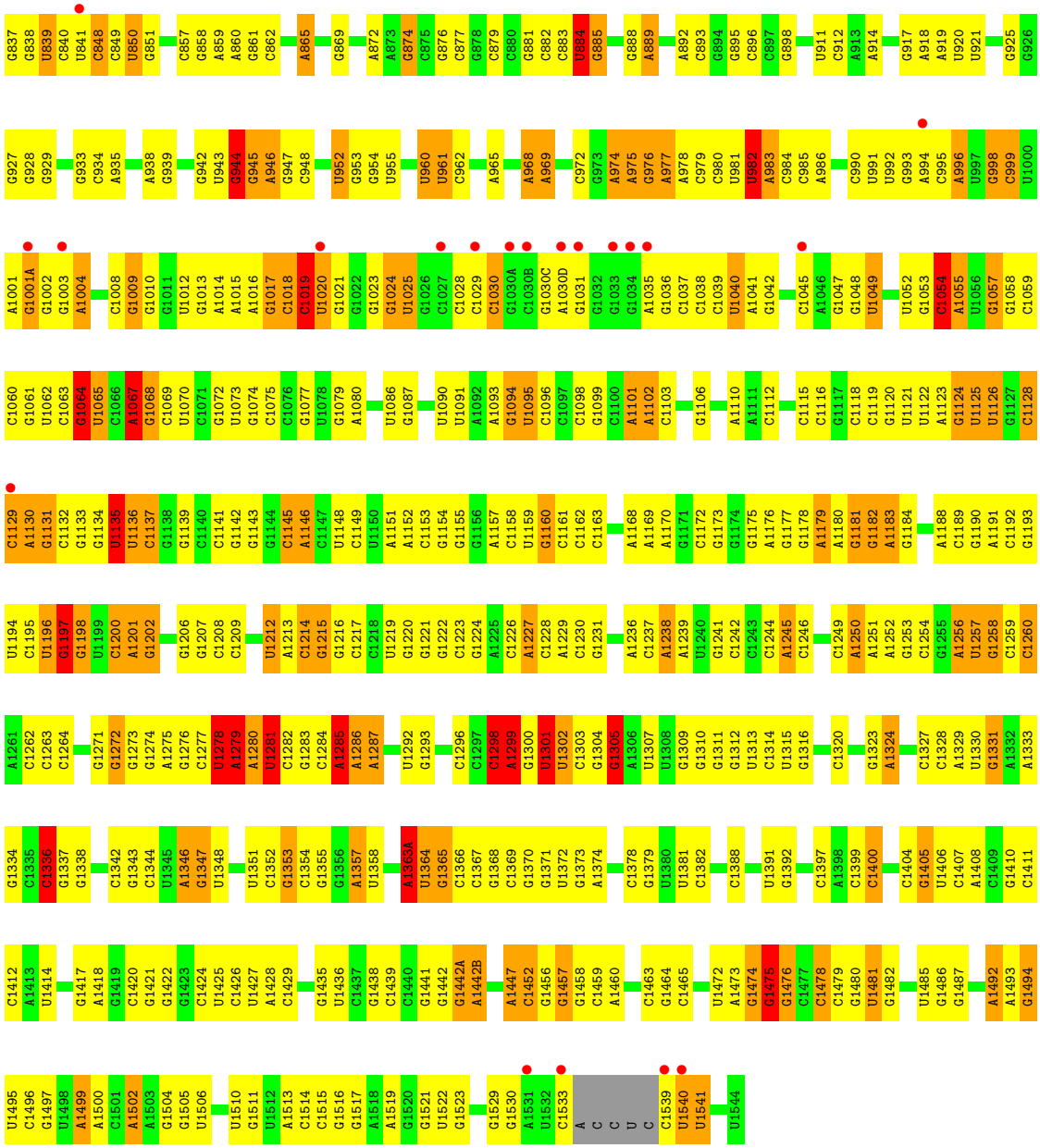
3 Residue-property plots (i)

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

- Molecule 1: 16S RIBOSOMAL RNA

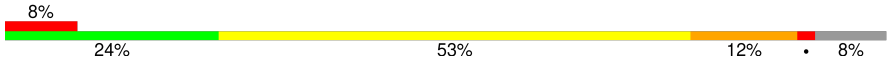
Chain A:

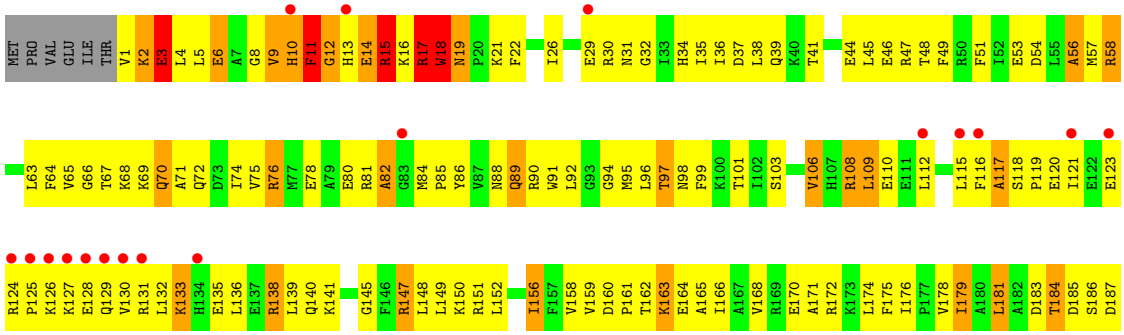


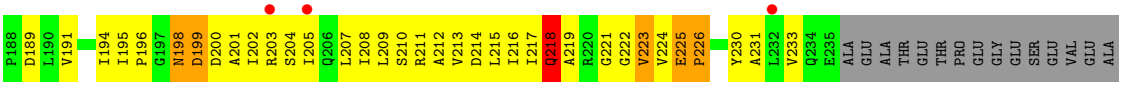


• Molecule 2: 30S RIBOSOMAL PROTEIN S2

Chain B:

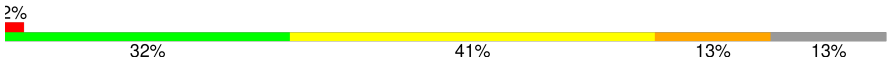


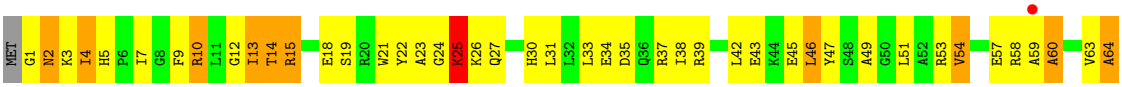


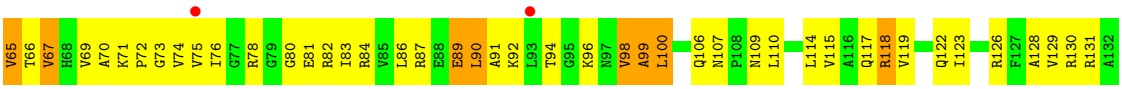


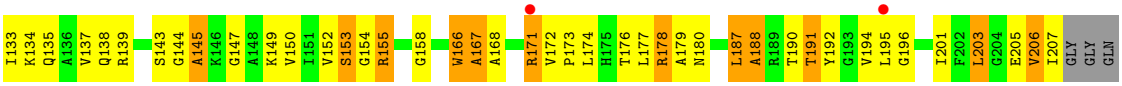
• Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain C:



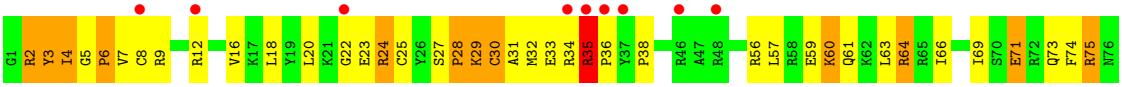


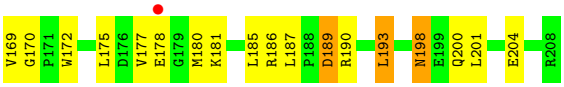




• Molecule 4: 30S RIBOSOMAL PROTEIN S4

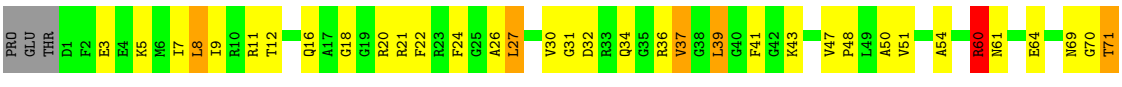
Chain D:

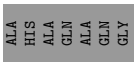




• Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain E:



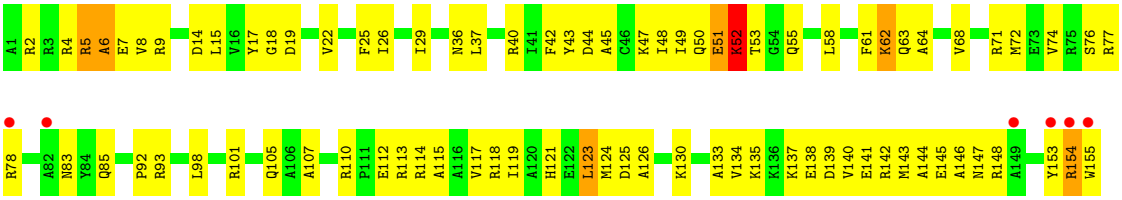


• Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain F:

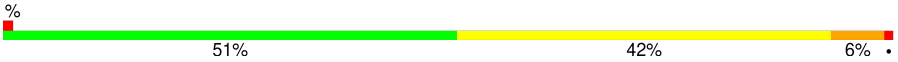
• Molecule 7: 30S RIBOSOMAL PROTEIN S7

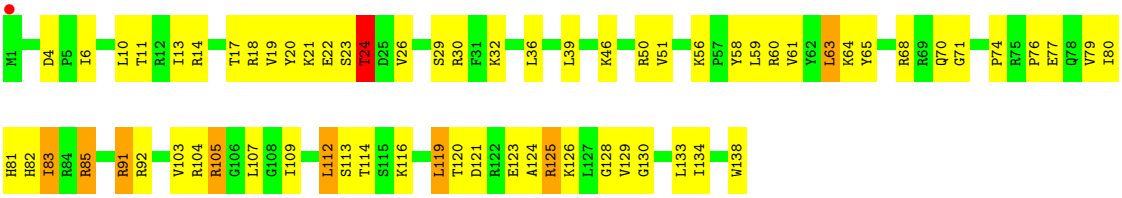
Chain G:



• Molecule 8: 30S RIBOSOMAL PROTEIN S8

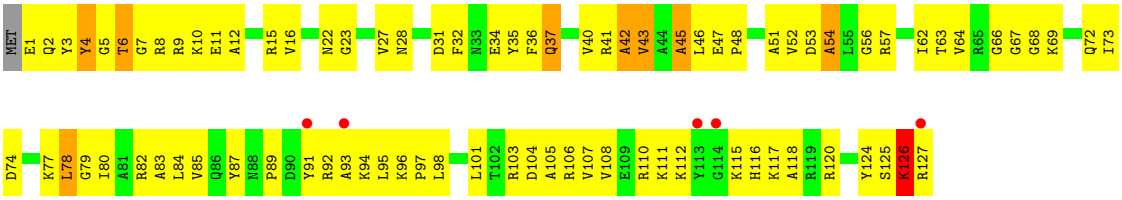
Chain H:





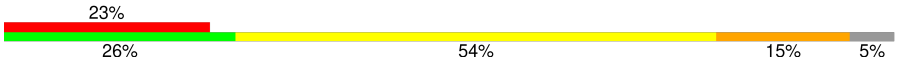
• Molecule 9: 30S RIBOSOMAL PROTEIN S9

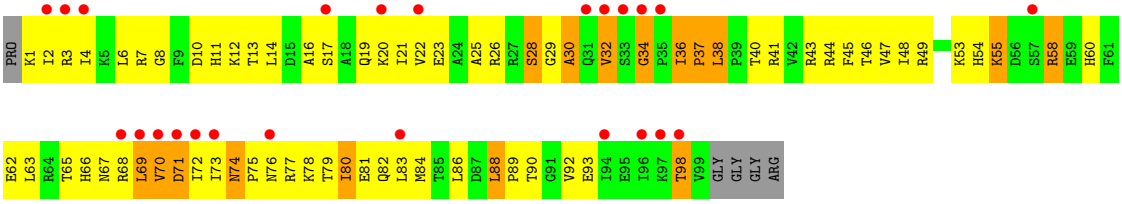
Chain I:



• Molecule 10: 30S RIBOSOMAL PROTEIN S10

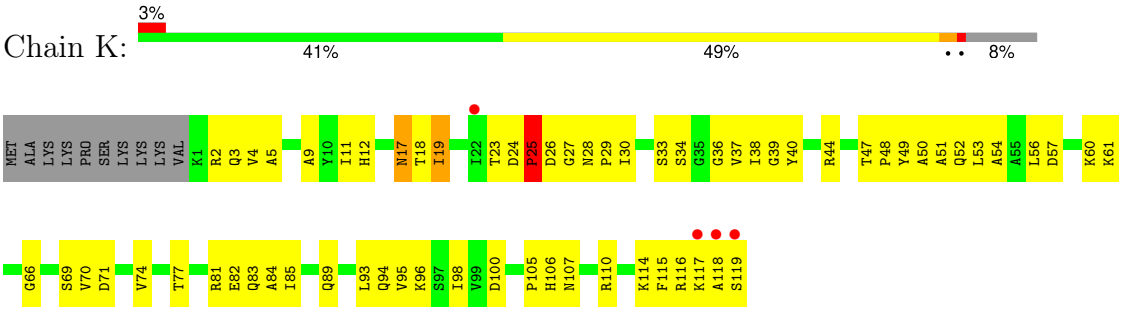
Chain J:





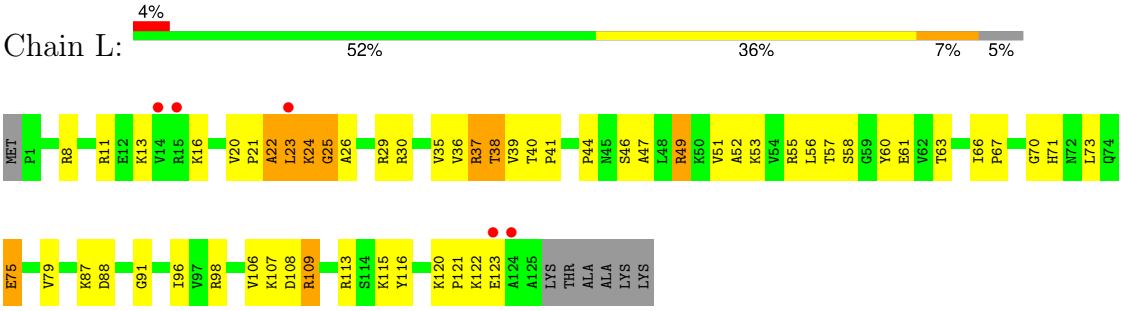
• Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain K:



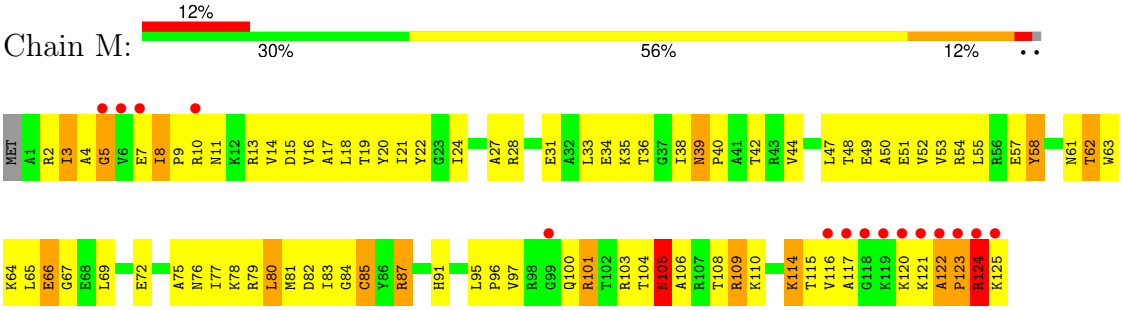
• Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain L:



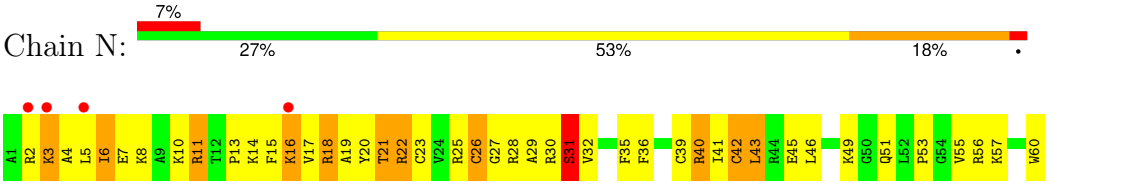
• Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain M:



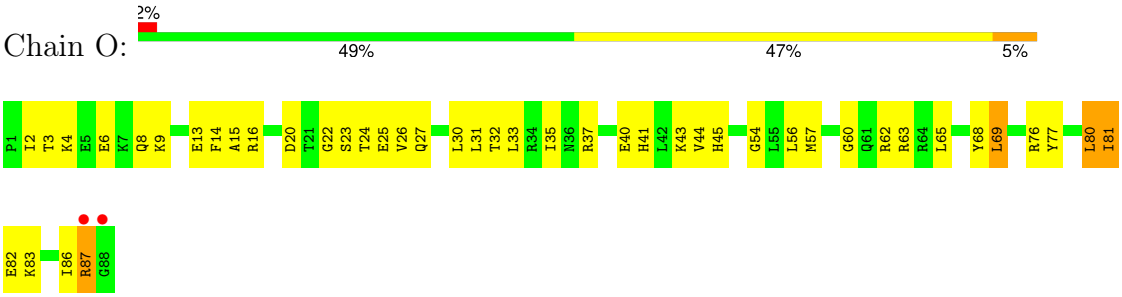
• Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z

Chain N:



• Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain O:



• Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain P: 52% 38% 6% 5%

M1 V2 K3 I4 R5 L6 R18 I19 V20 V21 R26 K27 R28 D29 G30 K31 Y32 I33 E34 Y38 Y39 D40 P41 R42 K43 T44 T45 W48 L49 K50 V51 D52 V53 E54 R55 W59 A64 T67 D68 T69 R72 L73 L74 R75 G78 V79 F80 R81 Q82 E83 A84

ARG GLU GLY ALA

• Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain Q: 5% 63% 28% 8%

P1 V4 K13 H14 Q15 K16 Q25 F26 P27 K33 R37 H44 D45 V55 I58 R62 P63 I64 S65 K66 R67 K68 R69 F70 R71 V72 L73 R74 L75 V76 E77 S78 G79 R80 R91 Q92 N93 Y94 Q95 S96 L97 S98 K99 R100 G101 G102 K103 A104

• Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain R: 3% 32% 45% 6% 17%

MET SER THR LYS ASN ALA LYS PRO LYS LYS GLU ALA GLN ARG ARG P1 S2 R3 K4 A5 K6 V7 T10 L11 G12 E13 R17 D18 Y19 R20 N21 V22 E23 V24 L25 K26 R27 F28 L29 S30 E31 T32 G33 R38 R39 R40 T41 G42 L43 S44 G45 K46 E47 Q48 R49 I50

T54 I55 K56 R57 A58 R59 I60 L61 G62 L63 L64 E68 V71 R72 K73

• Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain S: 7% 27% 52% 9% 12%

P1 R2 S3 L4 K5 K6 G7 V8 F9 V10 D11 L14 L15 E16 K17 V18 L19 E20 L21 N22 G25 E26 K27 R28 L29 I30 K31 T32 W33 S34 R35 R36 S37 T38 I39 V40 P41 E42 M43 V44 G45 H46 T47 I48 A49 V50 Y51 N52 G53 K54 Q55 H56 V57 I61 T62 E63 N64

M65 V66 K69 L70 F73 T76 R77 T78 Y79 R80 G81 HIS GLY LYS GLU ALA LYS ALA THR LYS LYS LYS

• Molecule 20: 30S RIBOSOMAL PROTEIN S20

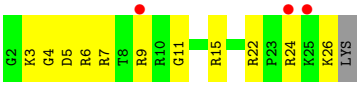
Chain T: 5% 55% 27% 11% 7%

MET ALA GLN LYS LYS PRO LYS R1 N2 L3 S4 A5 L6 K7 R10 Q11 L29 Q35 L36 E43 E44 K47 R50 L55 A60 S63 T64 L65 H66 K67 N68 A69 R72 R73 K74 S75 R76 L77 M78 R79 R82 Q83 E86 A87 A88 G89 A90 P91

L92 I93 G94 G95 G96 L97 S98 A99

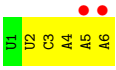
• Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain V: 12% 54% 42%



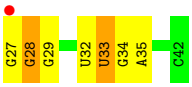
• Molecule 22: 5'-R(*UP*UP*CP*AP*AP*AP)-3'

Chain W:



• Molecule 23: 5'-R(*GP*GP*GP*AP*UP*UP*GP*AP*AP*AP*AP*UP*CP*CP*CP)-3'

Chain Z:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	401.65Å 401.65Å 175.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.90 39.77 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (40.00-2.90) 99.6 (39.77-2.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.04 (at 2.90Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.218 , 0.251 0.220 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	77.2	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 71.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	52505	wwPDB-VP
Average B, all atoms (Å^2)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.60% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ON0, K, MG, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.46	0/36362	0.76	66/56750 (0.1%)
2	B	0.36	0/1936	0.64	0/2611
3	C	0.40	0/1637	0.64	0/2207
4	D	0.38	0/1733	0.60	0/2318
5	E	0.47	0/1163	0.72	1/1566 (0.1%)
6	F	0.36	0/856	0.59	0/1154
7	G	0.37	0/1276	0.59	0/1709
8	H	0.44	0/1136	0.73	0/1527
9	I	0.37	0/1029	0.64	0/1378
10	J	0.38	0/808	0.66	0/1087
11	K	0.39	0/900	0.70	1/1213 (0.1%)
12	L	0.47	0/987	0.78	0/1322
13	M	0.34	0/1008	0.62	0/1347
14	N	0.46	0/501	0.76	0/664
15	O	0.38	0/745	0.61	0/992
16	P	0.43	0/717	0.70	0/965
17	Q	0.47	0/870	0.75	1/1159 (0.1%)
18	R	0.35	0/603	0.62	0/799
19	S	0.48	0/662	0.68	0/892
20	T	0.40	0/764	0.69	0/1006
21	V	0.53	0/213	0.59	0/279
22	W	0.43	0/137	0.65	0/211
23	Z	0.42	0/383	0.68	0/596
All	All	0.44	0/56426	0.73	69/83752 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	48	44

There are no bond length outliers.

The worst 5 of 69 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	944	G	N9-C1'-C2'	11.13	128.47	114.00
1	A	1064	G	N9-C1'-C2'	10.84	128.09	114.00
1	A	189(B)	C	N1-C1'-C2'	10.52	127.68	114.00
1	A	944	G	C5'-C4'-O4'	10.10	121.22	109.10
1	A	884	U	C2'-C3'-O3'	9.69	130.81	109.50

5 of 48 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	115	G	C4'
1	A	189(B)	C	C3',C1',C4'
1	A	189(E)	U	C3',C4'
1	A	196	A	C3'
1	A	246	A	C3',C1',C4'

5 of 44 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	108	G	Sidechain
1	A	12	U	Sidechain
1	A	189(B)	C	Sidechain
1	A	195	A	Sidechain
1	A	73	G	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32486	0	16403	937	0
2	B	1901	0	1954	226	0
3	C	1613	0	1680	206	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1703	0	1767	117	0
5	E	1147	0	1210	90	0
6	F	843	0	857	57	0
7	G	1257	0	1299	85	0
8	H	1116	0	1177	63	0
9	I	1011	0	1045	102	0
10	J	795	0	843	112	0
11	K	885	0	907	62	0
12	L	971	0	1059	71	0
13	M	997	0	1075	105	0
14	N	492	0	534	51	0
15	O	734	0	773	40	0
16	P	701	0	720	34	0
17	Q	857	0	932	38	0
18	R	597	0	670	68	0
19	S	648	0	675	91	0
20	T	762	0	862	43	0
21	V	209	0	221	12	0
22	W	123	0	66	8	0
23	Z	342	0	175	11	0
24	A	223	0	0	0	0
24	B	1	0	0	0	0
24	D	1	0	0	0	0
24	E	3	0	0	0	0
24	H	4	0	0	0	0
24	I	1	0	0	0	0
24	K	1	0	0	0	0
24	L	1	0	0	0	0
24	M	1	0	0	0	0
24	N	1	0	0	0	0
24	Q	1	0	0	0	0
24	T	1	0	0	0	0
24	Z	1	0	0	0	0
25	A	17	0	0	0	0
26	A	49	0	49	2	0
27	D	1	0	0	0	0
27	N	1	0	0	0	0
28	A	7	0	0	0	0
All	All	52505	0	36953	2412	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 27.

The worst 5 of 2412 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1029:C:H2'	1:A:1030:C:H5"	1.24	1.15
1:A:1023:G:H3'	1:A:1024:G:H5"	1.16	1.14
1:A:1101:A:H4'	1:A:1102:A:H5'	1.21	1.14
1:A:1271:G:H2'	1:A:1272:G:H5"	1.31	1.11
10:J:30:ALA:HB2	10:J:74:ASN:HD22	1.16	1.09

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
2	B	233/256 (91%)	166 (71%)	45 (19%)	22 (9%)	0 1
3	C	205/239 (86%)	145 (71%)	38 (18%)	22 (11%)	0 1
4	D	206/208 (99%)	172 (84%)	22 (11%)	12 (6%)	1 5
5	E	149/161 (92%)	139 (93%)	9 (6%)	1 (1%)	22 54
6	F	99/101 (98%)	86 (87%)	13 (13%)	0	100 100
7	G	153/155 (99%)	128 (84%)	18 (12%)	7 (5%)	2 9
8	H	136/138 (99%)	120 (88%)	12 (9%)	4 (3%)	4 18
9	I	125/128 (98%)	99 (79%)	14 (11%)	12 (10%)	0 1
10	J	97/104 (93%)	69 (71%)	15 (16%)	13 (13%)	0 0
11	K	117/129 (91%)	96 (82%)	18 (15%)	3 (3%)	5 20
12	L	123/132 (93%)	106 (86%)	10 (8%)	7 (6%)	1 5
13	M	123/126 (98%)	94 (76%)	17 (14%)	12 (10%)	0 1
14	N	58/60 (97%)	43 (74%)	7 (12%)	8 (14%)	0 0
15	O	86/88 (98%)	79 (92%)	5 (6%)	2 (2%)	6 23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	P	82/88 (93%)	76 (93%)	5 (6%)	1 (1%)	13	40
17	Q	102/104 (98%)	86 (84%)	9 (9%)	7 (7%)	1	3
18	R	71/88 (81%)	62 (87%)	7 (10%)	2 (3%)	5	19
19	S	79/92 (86%)	61 (77%)	12 (15%)	6 (8%)	1	2
20	T	97/106 (92%)	76 (78%)	12 (12%)	9 (9%)	0	1
21	V	23/26 (88%)	18 (78%)	4 (17%)	1 (4%)	2	10
All	All	2364/2529 (94%)	1921 (81%)	292 (12%)	151 (6%)	1	4

5 of 151 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	10	HIS
2	B	11	PHE
2	B	12	GLY
2	B	18	TRP
2	B	117	ALA

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	202/220 (92%)	174 (86%)	28 (14%)	3	10
3	C	160/188 (85%)	148 (92%)	12 (8%)	13	37
4	D	180/180 (100%)	168 (93%)	12 (7%)	16	43
5	E	115/122 (94%)	104 (90%)	11 (10%)	8	25
6	F	90/90 (100%)	88 (98%)	2 (2%)	52	81
7	G	126/126 (100%)	123 (98%)	3 (2%)	49	79
8	H	119/119 (100%)	110 (92%)	9 (8%)	13	36
9	I	98/99 (99%)	93 (95%)	5 (5%)	24	56
10	J	88/91 (97%)	84 (96%)	4 (4%)	27	61
11	K	90/99 (91%)	82 (91%)	8 (9%)	9	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	L	104/109 (95%)	99 (95%)	5 (5%)	25	58
13	M	100/101 (99%)	89 (89%)	11 (11%)	6	19
14	N	49/49 (100%)	42 (86%)	7 (14%)	3	10
15	O	79/79 (100%)	74 (94%)	5 (6%)	18	46
16	P	72/74 (97%)	65 (90%)	7 (10%)	8	25
17	Q	96/96 (100%)	90 (94%)	6 (6%)	18	46
18	R	64/77 (83%)	61 (95%)	3 (5%)	26	59
19	S	71/79 (90%)	67 (94%)	4 (6%)	21	52
20	T	76/82 (93%)	67 (88%)	9 (12%)	5	16
21	V	19/21 (90%)	19 (100%)	0	100	100
All	All	1998/2101 (95%)	1847 (92%)	151 (8%)	13	36

5 of 151 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	N	42	CYS
20	T	6	LEU
15	O	56	LEU
17	Q	37	ARG
20	T	93	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 63 such sidechains are listed below:

Mol	Chain	Res	Type
6	F	27	GLN
17	Q	15	GLN
9	I	30	GLN
15	O	70	GLN
19	S	46	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1510/1521 (99%)	262 (17%)	61 (4%)
22	W	5/6 (83%)	0	0
23	Z	15/16 (93%)	2 (13%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	1530/1543 (99%)	264 (17%)	61 (3%)

5 of 264 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	9	G
1	A	29	G
1	A	32	A
1	A	39	G
1	A	47	C

5 of 61 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	748	C
1	A	1346	A
1	A	974	A
1	A	1336	C
1	A	1475	G

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 260 ligands modelled in this entry, 259 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	$\#\|Z\| > 2$
26	ON0	A	2759	-	53,54,54	1.43	7 (13%)	75,80,80	0.80	3 (4%)

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
26	ON0	A	2759	-	-	6/20/105/105	0/6/6/6

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	2759	ON0	CBC-CBP	-4.55	1.41	1.50
26	A	2759	ON0	O6-CBP	3.87	1.48	1.41
26	A	2759	ON0	O4-CBP	3.60	1.47	1.42
26	A	2759	ON0	CBW-CBT	2.67	1.57	1.52
26	A	2759	ON0	CAO-CBC	2.48	1.43	1.39

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	A	2759	ON0	O1-CBT-CBW	2.43	113.59	107.42
26	A	2759	ON0	CBQ-O3'-C3'	-2.42	112.25	117.98
26	A	2759	ON0	OAV-CBM-CAQ	2.05	110.01	106.07

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	A	2759	ON0	CBW-CBT-O1-C1
26	A	2759	ON0	OAV-CBQ-O3'-C3'
26	A	2759	ON0	CBE-CBT-O1-C1
26	A	2759	ON0	NAA-CAQ-CBM-OAV
26	A	2759	ON0	NAA-CAQ-CBM-CBJ

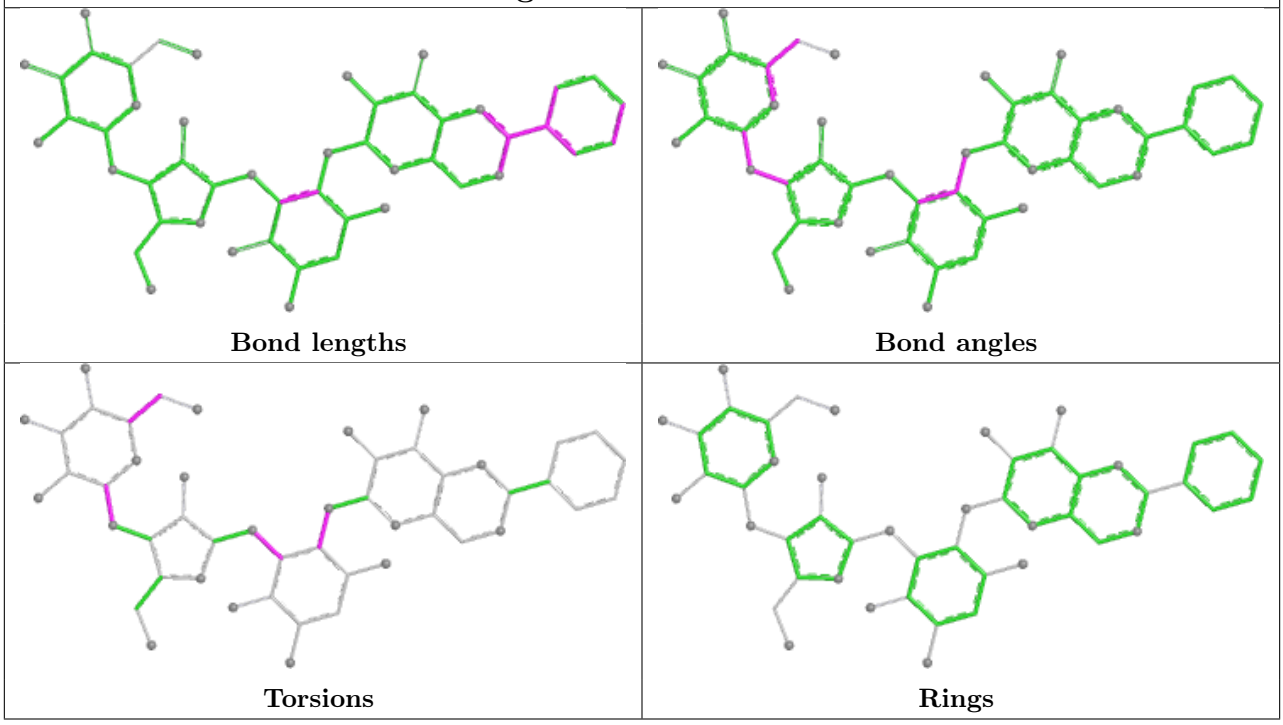
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	A	2759	ON0	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ON0 A 2759



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	1512/1521 (99%)	0.02	25 (1%)	70	69	44, 74, 145, 201	0
2	B	235/256 (91%)	0.34	21 (8%)	9	7	62, 110, 166, 189	0
3	C	207/239 (86%)	0.23	5 (2%)	59	56	62, 101, 148, 173	0
4	D	208/208 (100%)	0.13	10 (4%)	30	27	58, 85, 139, 194	0
5	E	151/161 (93%)	-0.15	0	100	100	44, 68, 102, 157	0
6	F	101/101 (100%)	0.05	2 (1%)	65	63	74, 104, 133, 159	0
7	G	155/155 (100%)	0.03	6 (3%)	39	35	65, 91, 146, 175	0
8	H	138/138 (100%)	-0.22	1 (0%)	87	87	45, 66, 93, 145	0
9	I	127/128 (99%)	0.39	5 (3%)	39	35	59, 110, 146, 196	0
10	J	99/104 (95%)	1.41	24 (24%)	0	0	55, 127, 184, 198	0
11	K	119/129 (92%)	0.23	4 (3%)	45	40	42, 80, 120, 179	0
12	L	125/132 (94%)	0.09	5 (4%)	38	33	41, 72, 110, 167	0
13	M	125/126 (99%)	0.88	15 (12%)	4	3	63, 94, 154, 187	0
14	N	60/60 (100%)	0.56	4 (6%)	17	13	61, 93, 133, 175	0
15	O	88/88 (100%)	0.05	2 (2%)	60	58	52, 81, 117, 171	0
16	P	84/88 (95%)	-0.09	0	100	100	52, 68, 101, 168	0
17	Q	104/104 (100%)	0.42	5 (4%)	30	27	40, 69, 132, 201	0
18	R	73/88 (82%)	0.26	3 (4%)	37	32	64, 87, 145, 196	0
19	S	81/92 (88%)	0.47	6 (7%)	14	11	72, 111, 153, 172	0
20	T	99/106 (93%)	0.14	5 (5%)	28	24	49, 74, 111, 148	0
21	V	25/26 (96%)	0.74	3 (12%)	4	3	63, 81, 121, 154	0
22	W	6/6 (100%)	0.87	2 (33%)	0	0	78, 87, 144, 171	0
23	Z	16/16 (100%)	0.60	1 (6%)	20	16	78, 111, 186, 191	0
All	All	3938/4072 (96%)	0.17	154 (3%)	39	35	40, 83, 151, 201	0

The worst 5 of 154 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	M	122	ALA	22.0
13	M	123	PRO	21.0
17	Q	104	ALA	20.2
11	K	119	SER	15.5
17	Q	103	LYS	12.4

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	MG	A	2703	1/1	0.29	0.67	87,87,87,87	0
24	MG	A	2750	1/1	0.30	0.94	97,97,97,97	0
24	MG	A	2758	1/1	0.36	0.40	93,93,93,93	0
25	K	A	2680	1/1	0.43	0.36	115,115,115,115	0
25	K	A	2669	1/1	0.44	0.32	113,113,113,113	0
24	MG	A	2591	1/1	0.45	0.31	83,83,83,83	0
24	MG	A	2744	1/1	0.45	0.77	85,85,85,85	0
24	MG	A	2721	1/1	0.46	0.17	88,88,88,88	0
24	MG	A	2617	1/1	0.46	0.96	119,119,119,119	0
24	MG	A	2718	1/1	0.47	0.52	75,75,75,75	0
24	MG	A	2747	1/1	0.49	0.31	66,66,66,66	0
24	MG	A	2660	1/1	0.50	0.47	125,125,125,125	0
24	MG	A	2575	1/1	0.50	0.64	91,91,91,91	0
24	MG	A	2743	1/1	0.51	0.52	84,84,84,84	0
24	MG	A	2739	1/1	0.52	0.27	83,83,83,83	0
24	MG	A	2748	1/1	0.53	0.23	80,80,80,80	0
24	MG	A	2722	1/1	0.54	0.91	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	MG	A	2592	1/1	0.54	0.13	77,77,77,77	0
24	MG	A	2749	1/1	0.55	0.19	66,66,66,66	0
24	MG	A	2734	1/1	0.57	0.23	92,92,92,92	0
24	MG	A	2746	1/1	0.60	0.20	69,69,69,69	0
24	MG	A	2554	1/1	0.60	0.43	78,78,78,78	0
24	MG	A	2717	1/1	0.61	0.46	83,83,83,83	0
24	MG	A	2623	1/1	0.62	0.11	69,69,69,69	0
24	MG	Z	1043	1/1	0.62	0.48	96,96,96,96	0
24	MG	A	2546	1/1	0.63	0.74	111,111,111,111	0
24	MG	A	2566	1/1	0.63	0.42	73,73,73,73	0
24	MG	H	1140	1/1	0.64	0.47	74,74,74,74	0
24	MG	A	2547	1/1	0.64	0.41	43,43,43,43	0
24	MG	A	2754	1/1	0.65	0.66	94,94,94,94	0
24	MG	A	2686	1/1	0.65	0.31	87,87,87,87	0
24	MG	A	2630	1/1	0.65	0.18	62,62,62,62	0
24	MG	A	2659	1/1	0.65	0.21	66,66,66,66	0
24	MG	A	2579	1/1	0.65	0.38	75,75,75,75	0
25	K	A	2670	1/1	0.65	0.26	105,105,105,105	0
25	K	A	2672	1/1	0.65	0.20	97,97,97,97	0
24	MG	A	2662	1/1	0.65	0.45	64,64,64,64	0
24	MG	A	2729	1/1	0.66	0.59	82,82,82,82	0
24	MG	A	2707	1/1	0.66	0.24	74,74,74,74	0
25	K	A	2681	1/1	0.66	0.18	118,118,118,118	0
24	MG	A	2553	1/1	0.67	1.03	94,94,94,94	0
25	K	A	2673	1/1	0.67	0.42	129,129,129,129	0
25	K	A	2683	1/1	0.67	0.12	111,111,111,111	0
25	K	A	2773	1/1	0.67	0.48	132,132,132,132	0
24	MG	A	2719	1/1	0.68	0.67	81,81,81,81	0
25	K	A	2674	1/1	0.68	0.22	114,114,114,114	0
24	MG	A	2613	1/1	0.68	0.84	73,73,73,73	0
24	MG	A	2715	1/1	0.68	0.42	74,74,74,74	0
24	MG	A	2694	1/1	0.68	0.17	94,94,94,94	0
24	MG	A	2666	1/1	0.68	0.45	96,96,96,96	0
24	MG	A	2628	1/1	0.69	0.40	68,68,68,68	0
24	MG	A	2624	1/1	0.69	0.14	59,59,59,59	0
24	MG	A	2736	1/1	0.69	0.28	82,82,82,82	0
24	MG	A	2637	1/1	0.69	0.21	70,70,70,70	0
24	MG	A	2665	1/1	0.69	0.33	82,82,82,82	0
24	MG	A	2648	1/1	0.69	0.14	52,52,52,52	0
24	MG	A	2704	1/1	0.70	0.21	83,83,83,83	0
24	MG	A	2723	1/1	0.70	0.38	90,90,90,90	0
24	MG	A	2564	1/1	0.71	0.20	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	MG	A	2556	1/1	0.71	0.23	102,102,102,102	0
24	MG	A	2658	1/1	0.71	0.15	59,59,59,59	0
24	MG	A	2593	1/1	0.71	0.37	89,89,89,89	0
24	MG	A	2714	1/1	0.72	0.43	91,91,91,91	0
24	MG	A	2753	1/1	0.72	0.17	80,80,80,80	0
24	MG	A	2652	1/1	0.72	0.19	66,66,66,66	0
24	MG	A	2555	1/1	0.73	0.87	68,68,68,68	0
24	MG	N	1062	1/1	0.73	0.37	111,111,111,111	0
24	MG	A	2634	1/1	0.74	0.18	66,66,66,66	0
24	MG	A	2548	1/1	0.74	0.31	63,63,63,63	0
24	MG	A	2757	1/1	0.74	0.40	92,92,92,92	0
25	K	A	2677	1/1	0.74	0.34	135,135,135,135	0
24	MG	A	2607	1/1	0.75	0.56	89,89,89,89	0
24	MG	A	2602	1/1	0.75	0.21	78,78,78,78	0
24	MG	A	2599	1/1	0.76	0.96	90,90,90,90	0
24	MG	A	2620	1/1	0.77	0.17	60,60,60,60	0
24	MG	A	2692	1/1	0.77	0.21	90,90,90,90	0
24	MG	A	2724	1/1	0.77	0.92	84,84,84,84	0
24	MG	H	1139	1/1	0.77	0.33	75,75,75,75	0
25	K	A	2676	1/1	0.77	0.13	100,100,100,100	0
24	MG	A	2661	1/1	0.78	0.81	75,75,75,75	0
24	MG	A	2737	1/1	0.78	1.23	100,100,100,100	0
24	MG	A	2767	1/1	0.78	0.39	66,66,66,66	0
24	MG	A	2752	1/1	0.79	0.21	67,67,67,67	0
24	MG	A	2731	1/1	0.79	0.34	77,77,77,77	0
24	MG	A	2551	1/1	0.79	0.19	60,60,60,60	0
24	MG	A	2728	1/1	0.80	0.23	80,80,80,80	0
24	MG	A	2651	1/1	0.80	0.18	69,69,69,69	0
24	MG	A	2691	1/1	0.80	0.73	73,73,73,73	0
24	MG	A	2275	1/1	0.80	0.71	69,69,69,69	0
24	MG	A	2650	1/1	0.80	0.17	55,55,55,55	0
24	MG	A	2576	1/1	0.81	0.36	75,75,75,75	0
24	MG	A	2745	1/1	0.81	0.20	57,57,57,57	0
24	MG	A	2577	1/1	0.81	0.22	45,45,45,45	0
24	MG	A	2633	1/1	0.81	0.16	92,92,92,92	0
24	MG	A	2578	1/1	0.81	0.34	53,53,53,53	0
24	MG	A	2654	1/1	0.81	0.29	63,63,63,63	0
24	MG	A	2627	1/1	0.81	0.13	63,63,63,63	0
24	MG	A	2636	1/1	0.82	0.20	71,71,71,71	0
24	MG	A	2695	1/1	0.82	0.21	76,76,76,76	0
24	MG	A	2655	1/1	0.82	0.23	57,57,57,57	0
24	MG	A	2567	1/1	0.82	0.37	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	MG	A	2586	1/1	0.82	0.27	70,70,70,70	0
24	MG	A	2545	1/1	0.83	0.13	64,64,64,64	0
24	MG	A	2619	1/1	0.83	0.23	54,54,54,54	0
24	MG	A	2760	1/1	0.83	0.50	73,73,73,73	0
24	MG	A	2549	1/1	0.83	0.14	57,57,57,57	0
24	MG	A	2563	1/1	0.83	0.20	86,86,86,86	0
24	MG	A	2550	1/1	0.83	0.25	60,60,60,60	0
24	MG	A	2687	1/1	0.83	0.16	65,65,65,65	0
24	MG	Q	1105	1/1	0.83	0.09	69,69,69,69	0
24	MG	A	2612	1/1	0.83	0.23	59,59,59,59	0
24	MG	A	2565	1/1	0.83	0.21	60,60,60,60	0
24	MG	A	2618	1/1	0.84	0.85	76,76,76,76	0
24	MG	A	2608	1/1	0.84	0.39	60,60,60,60	0
24	MG	A	2685	1/1	0.84	0.13	50,50,50,50	0
24	MG	A	2741	1/1	0.84	0.70	86,86,86,86	0
24	MG	A	2755	1/1	0.84	0.22	63,63,63,63	0
24	MG	A	2559	1/1	0.84	1.32	83,83,83,83	0
24	MG	A	2711	1/1	0.84	0.66	95,95,95,95	0
24	MG	A	2725	1/1	0.84	0.19	67,67,67,67	0
24	MG	A	2631	1/1	0.84	0.14	54,54,54,54	0
24	MG	A	2285	1/1	0.84	0.69	84,84,84,84	0
24	MG	A	2558	1/1	0.84	0.85	58,58,58,58	0
24	MG	L	1125	1/1	0.84	0.41	63,63,63,63	0
24	MG	A	2653	1/1	0.84	0.20	68,68,68,68	0
24	MG	A	2740	1/1	0.85	0.44	66,66,66,66	0
24	MG	A	2713	1/1	0.85	0.25	70,70,70,70	0
24	MG	H	1142	1/1	0.85	0.31	72,72,72,72	0
24	MG	A	2764	1/1	0.86	0.43	84,84,84,84	0
24	MG	A	2693	1/1	0.86	0.44	75,75,75,75	0
24	MG	B	1235	1/1	0.86	0.16	95,95,95,95	0
24	MG	T	1100	1/1	0.86	0.33	60,60,60,60	0
24	MG	D	1210	1/1	0.86	0.16	59,59,59,59	0
24	MG	A	2632	1/1	0.86	0.30	75,75,75,75	0
24	MG	A	2621	1/1	0.86	0.18	68,68,68,68	0
24	MG	A	2709	1/1	0.86	0.37	75,75,75,75	0
24	MG	A	2684	1/1	0.87	0.51	63,63,63,63	0
25	K	A	2678	1/1	0.87	0.26	102,102,102,102	0
24	MG	A	2699	1/1	0.87	0.18	78,78,78,78	0
24	MG	A	2629	1/1	0.87	0.17	53,53,53,53	0
24	MG	A	2649	1/1	0.87	0.19	54,54,54,54	0
24	MG	A	2625	1/1	0.87	0.12	49,49,49,49	0
24	MG	A	2580	1/1	0.88	0.22	115,115,115,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	MG	A	2611	1/1	0.88	0.45	51,51,51,51	0
24	MG	A	2643	1/1	0.88	0.15	55,55,55,55	0
24	MG	A	2573	1/1	0.88	0.10	57,57,57,57	0
24	MG	A	2701	1/1	0.88	0.16	86,86,86,86	0
24	MG	A	2283	1/1	0.88	0.34	72,72,72,72	0
24	MG	A	2732	1/1	0.88	0.39	87,87,87,87	0
24	MG	A	2615	1/1	0.88	0.27	60,60,60,60	0
24	MG	A	2605	1/1	0.88	0.13	43,43,43,43	0
24	MG	A	2282	1/1	0.88	1.04	82,82,82,82	0
24	MG	A	2768	1/1	0.88	0.52	83,83,83,83	0
24	MG	A	2663	1/1	0.89	0.36	70,70,70,70	0
24	MG	A	2705	1/1	0.89	0.40	77,77,77,77	0
24	MG	A	2569	1/1	0.89	0.35	55,55,55,55	0
24	MG	A	2751	1/1	0.89	0.20	64,64,64,64	0
24	MG	A	2708	1/1	0.89	0.97	82,82,82,82	0
24	MG	A	2639	1/1	0.89	0.64	65,65,65,65	0
24	MG	A	2552	1/1	0.89	0.36	46,46,46,46	0
25	K	A	2682	1/1	0.89	0.38	117,117,117,117	0
24	MG	A	2702	1/1	0.89	0.35	65,65,65,65	0
24	MG	A	2614	1/1	0.89	0.54	80,80,80,80	0
25	K	A	2671	1/1	0.90	0.22	90,90,90,90	0
24	MG	A	2667	1/1	0.90	0.22	108,108,108,108	0
24	MG	A	2641	1/1	0.90	0.21	49,49,49,49	0
24	MG	A	2279	1/1	0.90	0.65	80,80,80,80	0
24	MG	A	2756	1/1	0.90	0.23	83,83,83,83	0
24	MG	E	1152	1/1	0.90	0.68	71,71,71,71	0
24	MG	A	2277	1/1	0.91	0.83	69,69,69,69	0
24	MG	A	2710	1/1	0.91	0.58	76,76,76,76	0
24	MG	M	1126	1/1	0.91	0.13	55,55,55,55	0
24	MG	A	2771	1/1	0.91	0.87	89,89,89,89	0
24	MG	A	2772	1/1	0.91	0.27	95,95,95,95	0
24	MG	A	2664	1/1	0.91	0.64	69,69,69,69	0
24	MG	A	2598	1/1	0.91	0.31	66,66,66,66	0
25	K	A	2668	1/1	0.91	0.09	99,99,99,99	0
24	MG	A	2656	1/1	0.91	0.13	72,72,72,72	0
24	MG	A	2689	1/1	0.91	0.34	96,96,96,96	0
24	MG	A	2278	1/1	0.91	0.26	72,72,72,72	0
24	MG	A	2635	1/1	0.92	0.13	49,49,49,49	0
24	MG	A	2595	1/1	0.92	0.36	61,61,61,61	0
24	MG	A	2609	1/1	0.92	0.19	91,91,91,91	0
24	MG	A	2587	1/1	0.92	0.73	64,64,64,64	0
24	MG	A	2640	1/1	0.92	0.18	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	MG	A	2570	1/1	0.92	0.57	72,72,72,72	0
24	MG	A	2769	1/1	0.92	0.50	85,85,85,85	0
24	MG	A	2284	1/1	0.92	0.48	98,98,98,98	0
24	MG	A	2274	1/1	0.92	0.59	62,62,62,62	0
24	MG	A	2726	1/1	0.92	0.29	89,89,89,89	0
24	MG	A	2594	1/1	0.92	0.20	61,61,61,61	0
24	MG	A	2616	1/1	0.92	0.24	48,48,48,48	0
24	MG	A	2765	1/1	0.93	0.55	61,61,61,61	0
24	MG	A	2727	1/1	0.93	0.36	70,70,70,70	0
24	MG	K	1120	1/1	0.93	0.17	59,59,59,59	0
24	MG	A	2568	1/1	0.93	0.32	52,52,52,52	0
24	MG	A	2561	1/1	0.93	0.49	44,44,44,44	0
24	MG	A	2770	1/1	0.93	0.98	68,68,68,68	0
24	MG	A	2730	1/1	0.93	0.42	75,75,75,75	0
25	K	A	2679	1/1	0.93	0.49	120,120,120,120	0
24	MG	A	2276	1/1	0.93	0.39	74,74,74,74	0
24	MG	A	2742	1/1	0.93	0.44	60,60,60,60	0
24	MG	A	2281	1/1	0.93	0.77	72,72,72,72	0
24	MG	A	2761	1/1	0.93	0.93	86,86,86,86	0
24	MG	A	2604	1/1	0.93	0.41	63,63,63,63	0
24	MG	A	2762	1/1	0.94	0.57	53,53,53,53	0
24	MG	A	2638	1/1	0.94	0.19	68,68,68,68	0
24	MG	E	1151	1/1	0.94	0.38	72,72,72,72	0
24	MG	A	2597	1/1	0.94	0.29	53,53,53,53	0
24	MG	A	2720	1/1	0.94	0.58	90,90,90,90	0
24	MG	A	2583	1/1	0.94	0.54	59,59,59,59	0
24	MG	A	2589	1/1	0.94	0.24	55,55,55,55	0
24	MG	A	2590	1/1	0.94	0.24	80,80,80,80	0
24	MG	A	2610	1/1	0.94	0.23	55,55,55,55	0
24	MG	A	2557	1/1	0.94	0.47	67,67,67,67	0
24	MG	A	2738	1/1	0.95	0.31	67,67,67,67	0
24	MG	A	2646	1/1	0.95	0.17	50,50,50,50	0
25	K	A	2675	1/1	0.95	0.19	105,105,105,105	0
24	MG	A	2584	1/1	0.95	0.28	54,54,54,54	0
24	MG	A	2600	1/1	0.95	0.14	60,60,60,60	0
24	MG	A	2688	1/1	0.95	0.20	79,79,79,79	0
24	MG	A	2601	1/1	0.95	0.44	61,61,61,61	0
24	MG	E	1153	1/1	0.95	0.38	57,57,57,57	0
24	MG	A	2571	1/1	0.95	0.47	57,57,57,57	0
24	MG	A	2572	1/1	0.95	0.39	71,71,71,71	0
24	MG	A	2645	1/1	0.95	0.10	34,34,34,34	0
24	MG	A	2706	1/1	0.95	0.42	67,67,67,67	0

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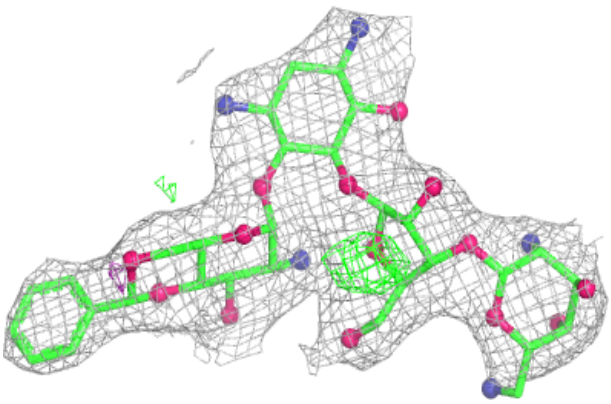
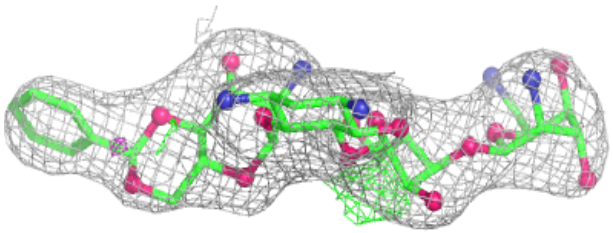
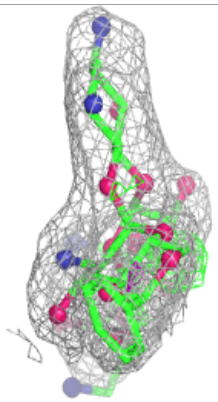
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	ON0	A	2759	49/49	0.95	0.21	56,64,79,80	0
24	MG	H	1141	1/1	0.96	0.43	70,70,70,70	0
24	MG	A	2763	1/1	0.96	0.55	56,56,56,56	0
24	MG	A	2733	1/1	0.96	0.63	63,63,63,63	0
24	MG	A	2581	1/1	0.96	0.47	59,59,59,59	0
24	MG	A	2716	1/1	0.96	0.71	77,77,77,77	0
24	MG	A	2700	1/1	0.96	0.12	61,61,61,61	0
24	MG	A	2596	1/1	0.96	0.28	45,45,45,45	0
24	MG	A	2606	1/1	0.96	0.23	49,49,49,49	0
24	MG	A	2698	1/1	0.96	0.08	66,66,66,66	0
24	MG	A	2647	1/1	0.97	0.28	35,35,35,35	0
24	MG	A	2603	1/1	0.97	0.89	63,63,63,63	0
24	MG	A	2657	1/1	0.97	0.30	28,28,28,28	0
24	MG	A	2280	1/1	0.97	0.45	72,72,72,72	0
24	MG	A	2626	1/1	0.97	0.07	49,49,49,49	0
24	MG	A	2588	1/1	0.97	0.31	55,55,55,55	0
24	MG	A	2697	1/1	0.97	0.20	99,99,99,99	0
24	MG	I	1128	1/1	0.97	0.34	128,128,128,128	0
24	MG	A	2562	1/1	0.97	0.43	53,53,53,53	0
24	MG	A	2622	1/1	0.97	0.12	66,66,66,66	0
24	MG	A	2582	1/1	0.97	0.43	56,56,56,56	0
24	MG	A	2766	1/1	0.98	0.75	60,60,60,60	0
24	MG	A	2735	1/1	0.98	0.76	69,69,69,69	0
24	MG	A	2696	1/1	0.98	0.30	41,41,41,41	0
24	MG	A	2712	1/1	0.98	0.13	84,84,84,84	0
24	MG	A	2690	1/1	0.98	0.15	36,36,36,36	0
24	MG	A	2585	1/1	0.98	0.39	56,56,56,56	0
24	MG	A	2574	1/1	0.99	0.18	40,40,40,40	0
24	MG	A	2644	1/1	0.99	0.09	26,26,26,26	0
24	MG	A	2560	1/1	0.99	0.51	45,45,45,45	0
24	MG	A	2642	1/1	0.99	0.25	51,51,51,51	0
27	ZN	D	1209	1/1	0.99	0.28	103,103,103,103	0
27	ZN	N	1061	1/1	0.99	0.12	98,98,98,98	0

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

Electron density around ON0 A 2759: $2mF_o$-DF_c (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)	
	

6.5 Other polymers (i)

There are no such residues in this entry.