



wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 12:25 pm BST

PDB ID : 1XNQ
Title : Structure of an Inosine-Adenine Wobble Base Pair Complex in the Context of the Decoding Center
Authors : Murphy, F.V.; Ramakrishnan, V.
Deposited on : 2004-10-05
Resolution : 3.05 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

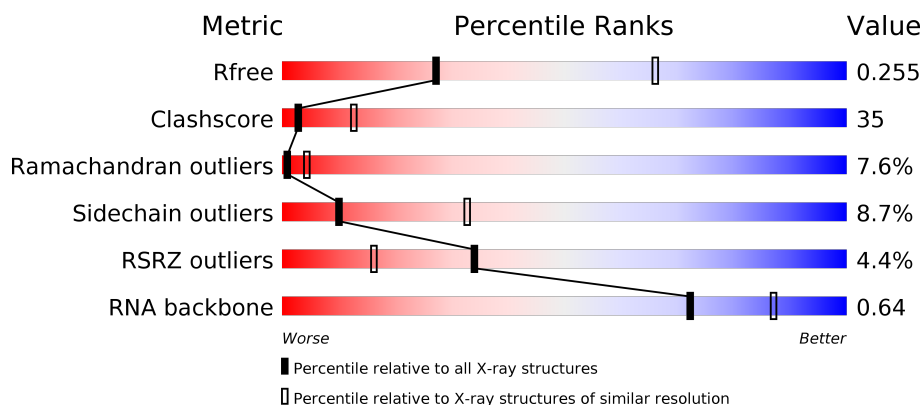
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.05 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.



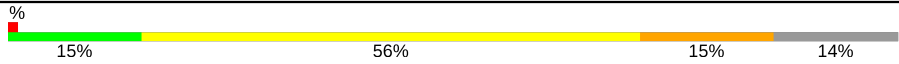

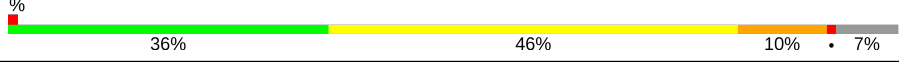
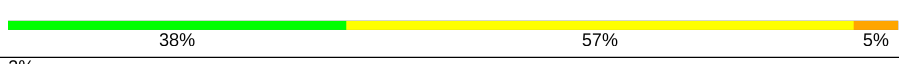
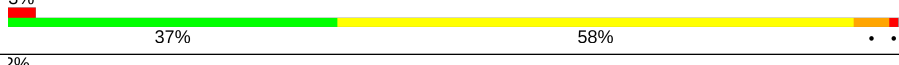

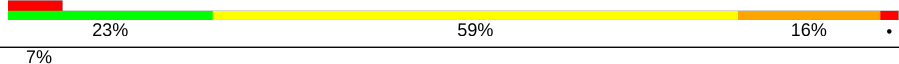
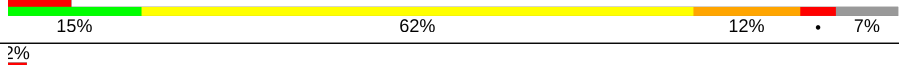
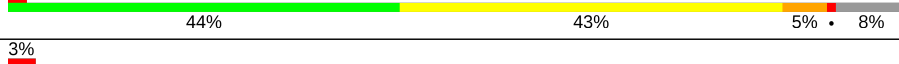
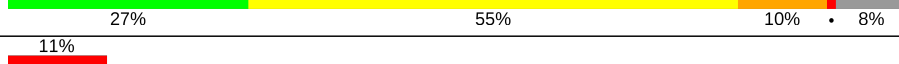
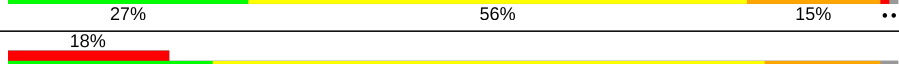

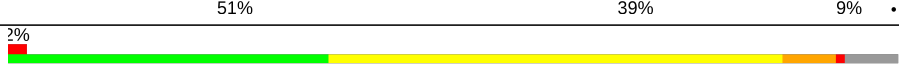
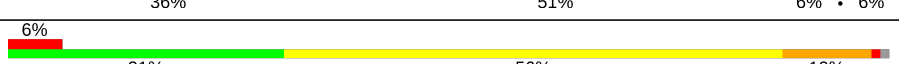
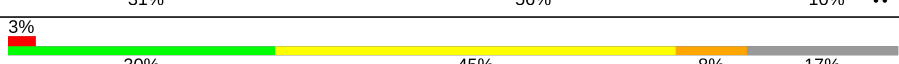
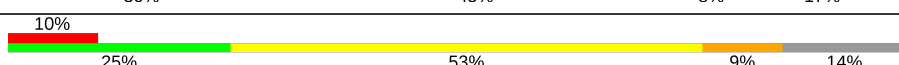
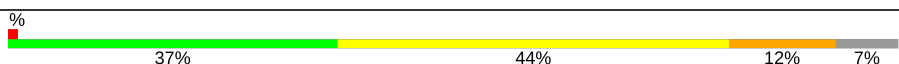
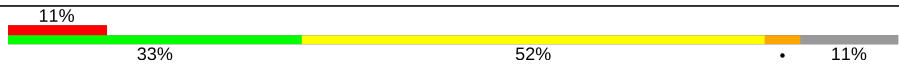

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)
RNA backbone	3102	1036 (3.32-2.80)

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	A	1522	<div> <div>5%</div> <div> <div></div> <div>32%</div> <div>53%</div> <div>12%</div> <div>..</div> </div> </div>
2	X	11	<div> <div>64%</div> <div>36%</div> </div>
3	W	4	<div> <div>75%</div> <div>25%</div> </div>
4	B	256	<div> <div>2%</div> <div> <div></div> <div>21%</div> <div>55%</div> <div>13%</div> <div>•</div> <div>9%</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	C	239	
6	D	209	
7	E	162	
8	F	101	
9	G	156	
10	H	138	
11	I	128	
12	J	105	
13	K	129	
14	L	135	
15	M	126	
16	N	61	
17	O	89	
18	P	88	
19	Q	105	
20	R	88	
21	S	93	
22	T	106	
23	V	27	

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
25	MG	A	1575	-	-	-	X
25	MG	A	1594	-	-	-	X
25	MG	A	467	-	-	-	X
25	MG	X	502	-	-	-	X

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 52076 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
1	A	1507	Total	C	N	O	P	0	0	0
			32380	14414	5990	10470	1506			

- Molecule 2 is a RNA chain called Anticodon tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	11	Total	C	N	O	P	0	0	0
			232	105	43	74	10			

- Molecule 3 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	W	4	Total	C	N	O	P	0	0	0
			84	39	18	24	3			

- Molecule 4 is a protein called Ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			

- Molecule 5 is a protein called Ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

- Molecule 6 is a protein called Ribosomal protein S4.

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

- Molecule 7 is a protein called Ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	150	Total	C	N	O	S	0	0	0
			1146	724	217	201	4			

- Molecule 8 is a protein called Ribosomal protein S6.

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

- Molecule 9 is a protein called Ribosomal protein S7.

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

- Molecule 10 is a protein called Ribosomal protein S8.

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

- Molecule 11 is a protein called Ribosomal protein S9.

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

- Molecule 12 is a protein called Ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	J	98	Total	C	N	O	S	0	0	0
			792	498	156	137	1			

- Molecule 13 is a protein called Ribosomal protein S11.

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

- Molecule 14 is a protein called Ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	L	124	Total	C	N	O	S	0	0	0
			970	611	195	163	1			

- Molecule 15 is a protein called Ribosomal protein S13.

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

- Molecule 16 is a protein called Ribosomal protein S14.

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

- Molecule 17 is a protein called Ribosomal protein S15.

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

- Molecule 18 is a protein called Ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	P	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			

- Molecule 19 is a protein called Ribosomal protein S17.

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

- Molecule 20 is a protein called Ribosomal protein S18.

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

- Molecule 21 is a protein called Ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	S	80	Total	C	N	O	S	0	0	0
			647	414	119	112	2			

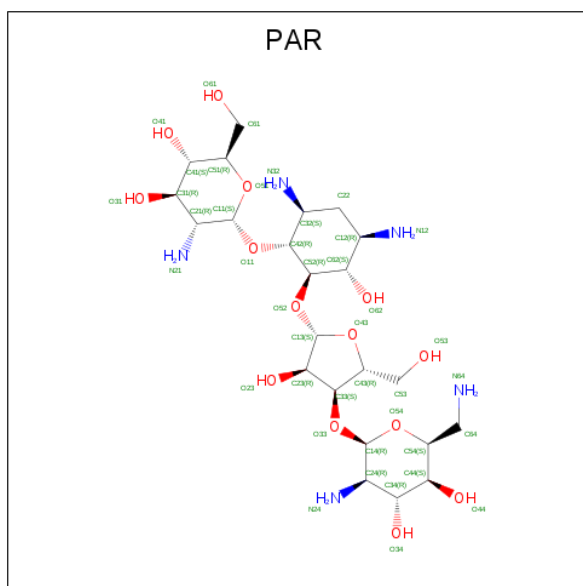
- Molecule 22 is a protein called Ribosomal protein S20.

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

- Molecule 23 is a protein called Ribosomal protein THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
23	V	24	Total	C	N	O	0	0	0
			208	128	50	30			

- Molecule 24 is PAROMOMYCIN (three-letter code: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	0
			42	23	5	14		

- Molecule 25 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	X	2	Total	Mg	0	0
			2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	J	1	Total 1	Mg 1	0	0
25	A	104	Total 104	Mg 104	0	0

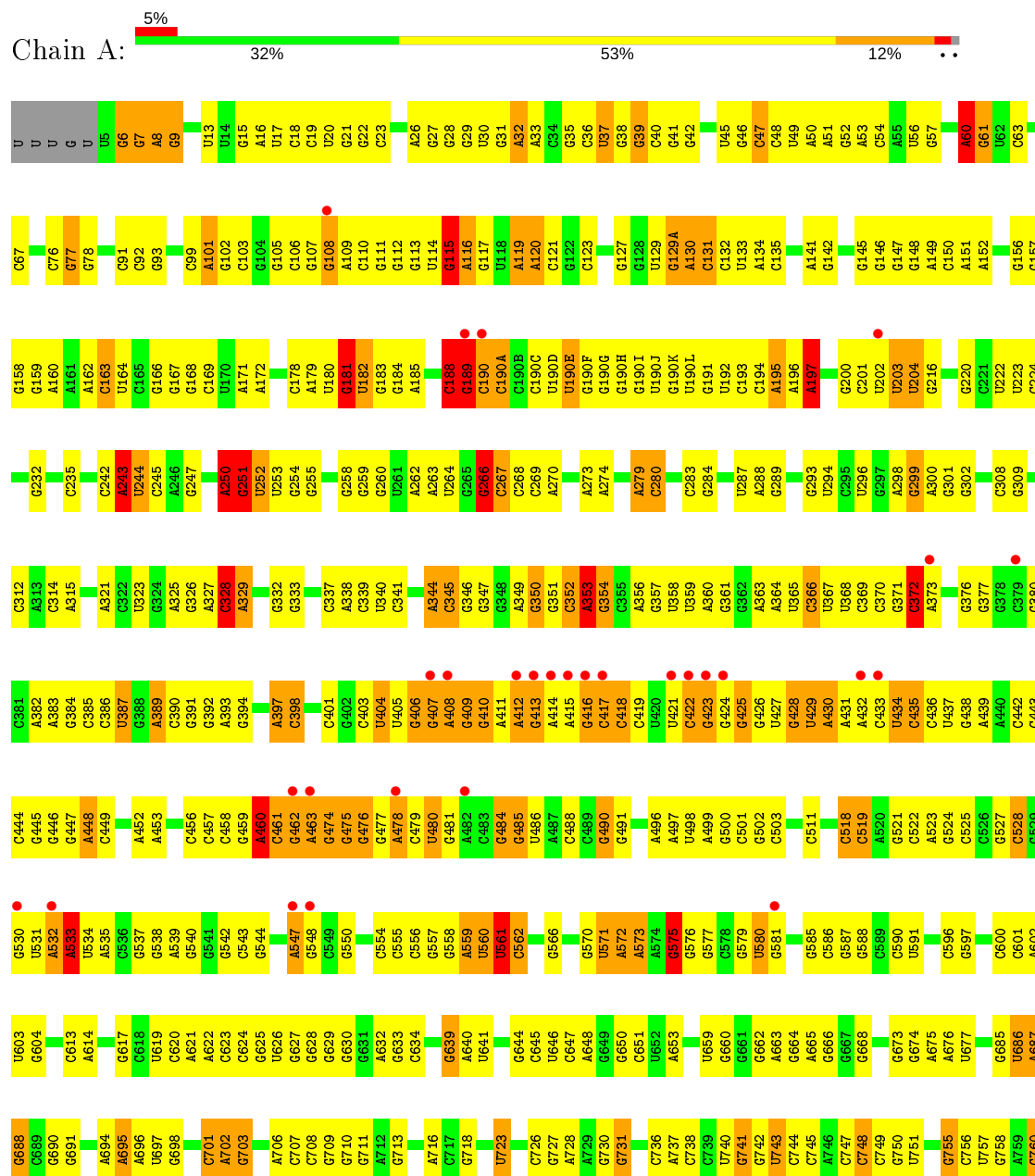
- Molecule 26 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

3 Residue-property plots

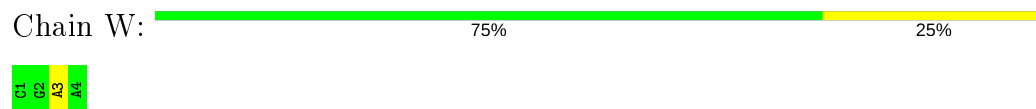
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: 16S ribosomal RNA

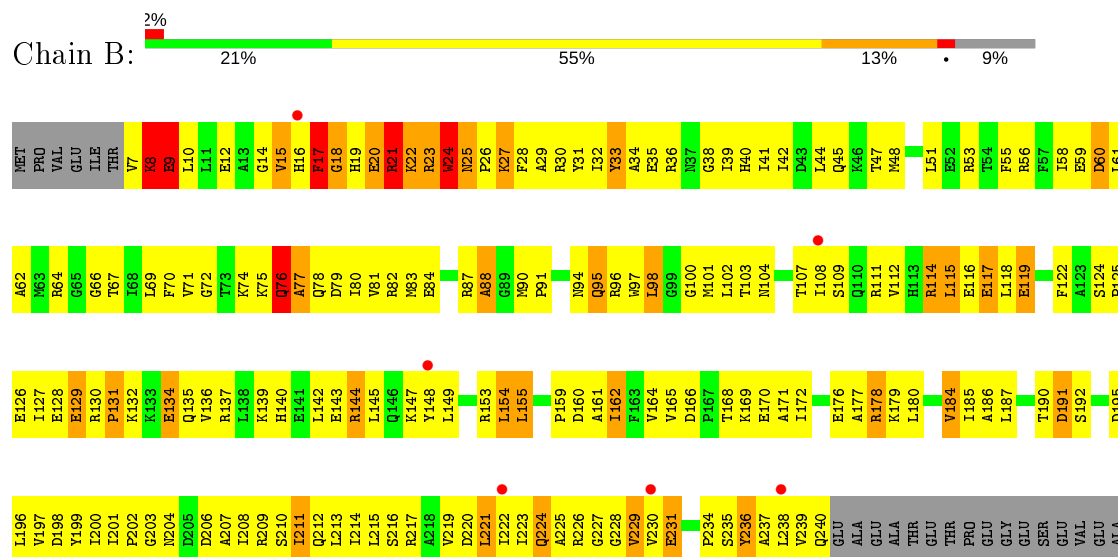




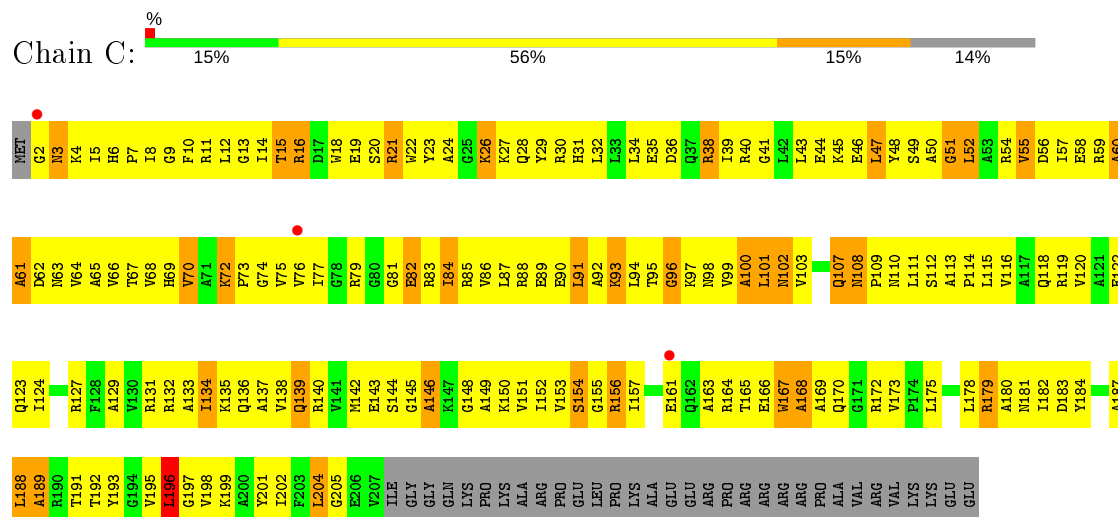
- Molecule 3: mRNA



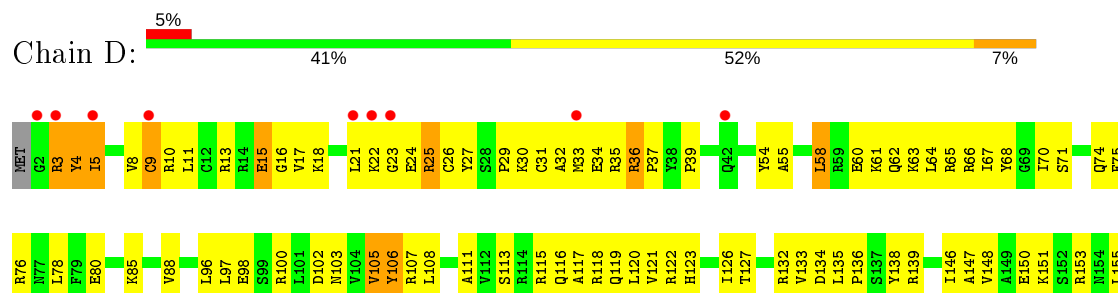
- Molecule 4: Ribosomal protein S2

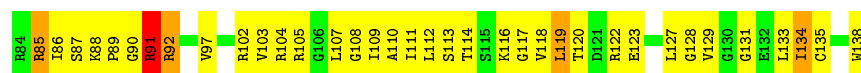


- Molecule 5: Ribosomal protein S3

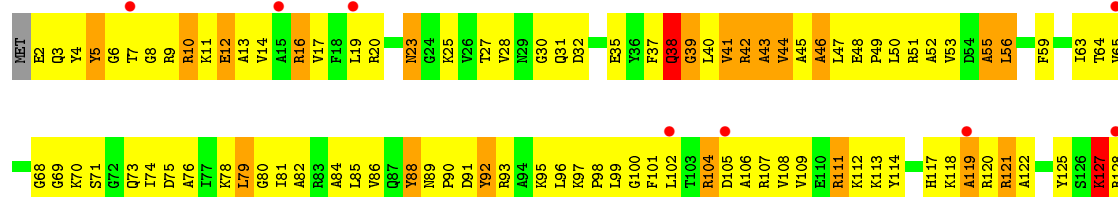


- Molecule 6: Ribosomal protein S4

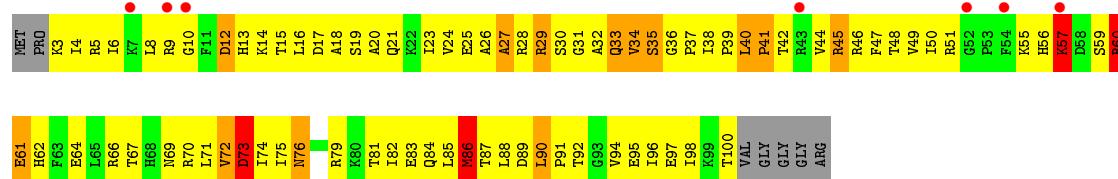
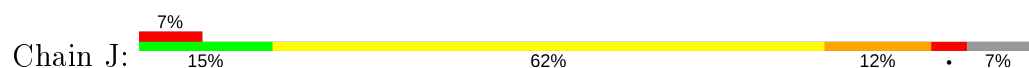




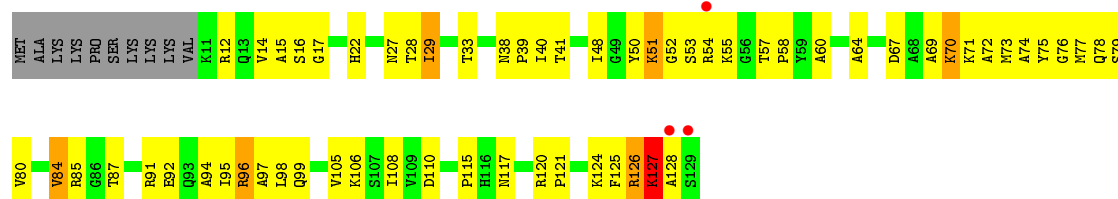
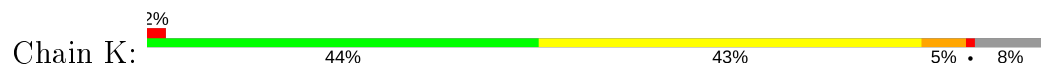
- Molecule 11: Ribosomal protein S9



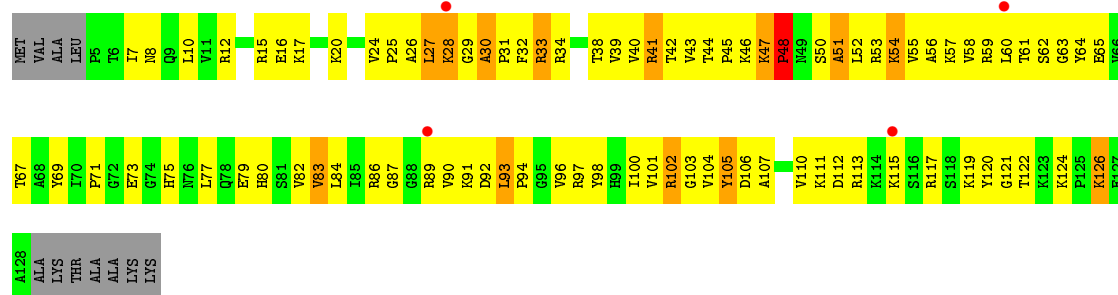
- Molecule 12: Ribosomal protein S10



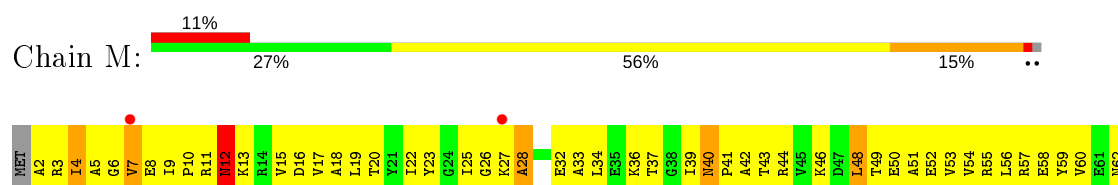
- Molecule 13: Ribosomal protein S11



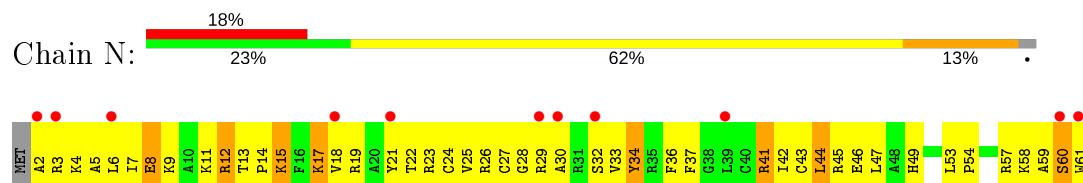
- Molecule 14: Ribosomal protein S12



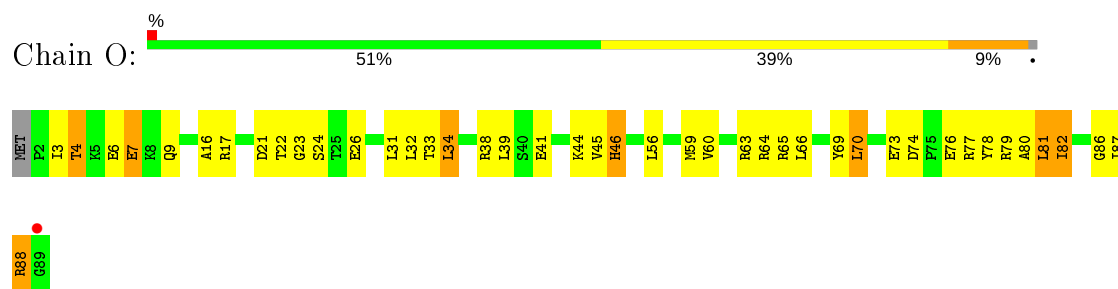
- Molecule 15: Ribosomal protein S13



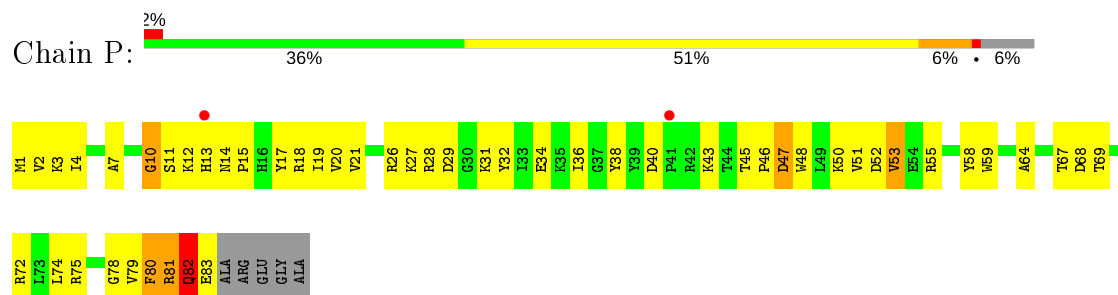
- Molecule 16: Ribosomal protein S14



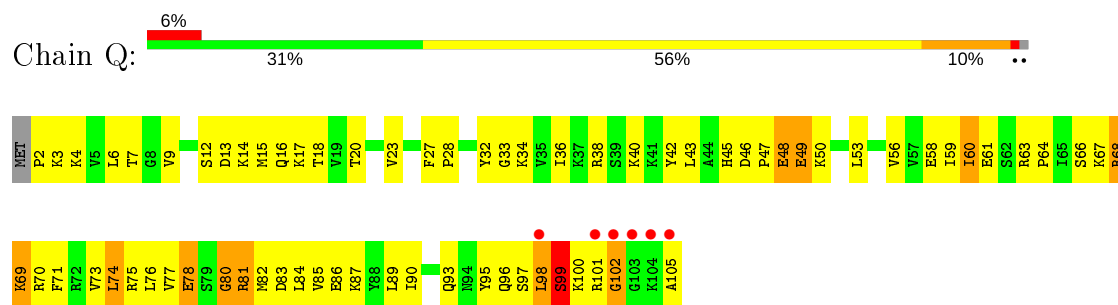
- Molecule 17: Ribosomal protein S15



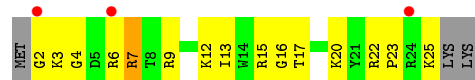
- Molecule 18: Ribosomal protein S16



- Molecule 19: Ribosomal protein S17



- Molecule 20: Ribosomal protein S18



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	401.13Å 401.13Å 175.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	99.00 – 3.05 283.65 – 2.98	Depositor EDS
% Data completeness (in resolution range)	89.6 (99.00-3.05) 88.7 (283.65-2.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.85 (at 2.96Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.228 , 0.270 0.214 , 0.255	Depositor DCC
R_{free} test set	13849 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	73.5	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 82.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	52076	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.58% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.53	2/36244 (0.0%)	0.75	37/56567 (0.1%)
2	X	0.54	0/258	0.83	0/398
3	W	0.39	0/94	0.71	0/145
4	B	0.33	0/1935	0.62	0/2609
5	C	0.37	0/1636	0.64	1/2205 (0.0%)
6	D	0.37	0/1733	0.65	0/2318
7	E	0.44	0/1162	0.73	0/1564
8	F	0.32	0/856	0.60	0/1154
9	G	0.35	0/1276	0.62	1/1709 (0.1%)
10	H	0.42	0/1136	0.75	0/1527
11	I	0.35	0/1029	0.63	0/1378
12	J	0.36	0/805	0.68	1/1082 (0.1%)
13	K	0.40	0/900	0.63	0/1213
14	L	0.42	0/986	0.74	0/1320
15	M	0.34	0/1008	0.65	0/1347
16	N	0.42	0/501	0.70	0/664
17	O	0.35	0/745	0.57	0/992
18	P	0.45	0/716	0.76	0/963
19	Q	0.45	0/870	0.75	0/1159
20	R	0.33	0/603	0.61	0/799
21	S	0.30	0/661	0.61	0/890
22	T	0.40	0/764	0.68	0/1006
23	V	0.42	0/212	0.65	0/277
All	All	0.48	2/56130 (0.0%)	0.72	40/83286 (0.0%)

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	3	42

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1361	G	C3'-O3'	5.55	1.50	1.42
1	A	1361	G	O3'-P	5.09	1.67	1.61

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1498	U	C2'-C3'-O3'	10.20	131.94	109.50
1	A	115	G	C2'-C3'-O3'	9.68	130.79	109.50
1	A	243	A	C2'-C3'-O3'	9.25	129.85	109.50
1	A	559	A	C2'-C3'-O3'	8.95	129.20	109.50
1	A	575	G	C2'-C3'-O3'	8.79	128.84	109.50

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	243	A	C3'
1	A	1498	U	C3'
1	A	1528	U	C3'

5 of 42 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	108	G	Sidechain
1	A	189	G	Sidechain
1	A	197	A	Sidechain
1	A	37	U	Sidechain
1	A	77	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	A	32380	0	16346	1153	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	X	232	0	120	4	0
3	W	84	0	46	1	0
4	B	1900	0	1951	274	0
5	C	1612	0	1677	274	0
6	D	1703	0	1764	153	0
7	E	1146	0	1207	118	0
8	F	843	0	857	68	0
9	G	1257	0	1296	110	0
10	H	1116	0	1177	112	0
11	I	1011	0	1043	124	0
12	J	792	0	835	151	1
13	K	885	0	904	77	0
14	L	970	0	1057	119	0
15	M	997	0	1072	124	0
16	N	492	0	529	66	0
17	O	734	0	771	54	0
18	P	700	0	720	66	0
19	Q	857	0	930	84	0
20	R	597	0	668	68	0
21	S	647	0	673	88	0
22	T	762	0	856	72	0
23	V	208	0	221	16	0
24	A	42	0	45	2	0
25	A	104	0	0	0	0
25	J	1	0	0	0	0
25	X	2	0	0	0	0
26	D	1	0	0	0	0
26	N	1	0	0	0	0
All	All	52076	0	36765	3117	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 35.

The worst 5 of 3117 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:243:A:H4'	1:A:244:U:H5'	1.30	1.13
12:J:45:ARG:HH11	12:J:45:ARG:HB3	0.99	1.13
14:L:47:LYS:HB3	14:L:48:PRO:HD3	1.32	1.12
6:D:151:LYS:H	6:D:151:LYS:HD2	1.08	1.11
6:D:36:ARG:H	6:D:37:PRO:HD3	1.14	1.10

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:79:ARG:NE	12:J:79:ARG:NE[8_665]	2.15	0.05

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	
4	B	232/256 (91%)	154 (66%)	52 (22%)	26 (11%)	0	2
5	C	204/239 (85%)	132 (65%)	48 (24%)	24 (12%)	0	1
6	D	206/209 (99%)	160 (78%)	37 (18%)	9 (4%)	2	12
7	E	148/162 (91%)	125 (84%)	17 (12%)	6 (4%)	3	14
8	F	99/101 (98%)	75 (76%)	19 (19%)	5 (5%)	2	10
9	G	153/156 (98%)	120 (78%)	27 (18%)	6 (4%)	3	15
10	H	136/138 (99%)	113 (83%)	18 (13%)	5 (4%)	3	16
11	I	125/128 (98%)	88 (70%)	23 (18%)	14 (11%)	0	2
12	J	96/105 (91%)	61 (64%)	23 (24%)	12 (12%)	0	1
13	K	117/129 (91%)	90 (77%)	22 (19%)	5 (4%)	2	13
14	L	122/135 (90%)	92 (75%)	18 (15%)	12 (10%)	0	2
15	M	123/126 (98%)	88 (72%)	21 (17%)	14 (11%)	0	1
16	N	58/61 (95%)	38 (66%)	17 (29%)	3 (5%)	2	10
17	O	86/89 (97%)	70 (81%)	11 (13%)	5 (6%)	1	8
18	P	81/88 (92%)	61 (75%)	16 (20%)	4 (5%)	2	11
19	Q	102/105 (97%)	80 (78%)	15 (15%)	7 (7%)	1	5
20	R	71/88 (81%)	53 (75%)	13 (18%)	5 (7%)	1	5
21	S	78/93 (84%)	50 (64%)	22 (28%)	6 (8%)	1	4
22	T	97/106 (92%)	71 (73%)	17 (18%)	9 (9%)	0	3

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	V	22/27 (82%)	16 (73%)	5 (23%)	1 (4%)	2	12
All	All	2356/2541 (93%)	1737 (74%)	441 (19%)	178 (8%)	1	4

5 of 178 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	B	8	LYS
4	B	20	GLU
4	B	21	ARG
4	B	24	TRP
4	B	77	ALA

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	
4	B	202/220 (92%)	178 (88%)	24 (12%)	5	18
5	C	160/188 (85%)	144 (90%)	16 (10%)	7	25
6	D	180/181 (99%)	166 (92%)	14 (8%)	12	37
7	E	115/123 (94%)	99 (86%)	16 (14%)	3	13
8	F	90/90 (100%)	88 (98%)	2 (2%)	52	76
9	G	126/127 (99%)	121 (96%)	5 (4%)	31	62
10	H	119/119 (100%)	109 (92%)	10 (8%)	11	34
11	I	98/99 (99%)	82 (84%)	16 (16%)	2	9
12	J	87/92 (95%)	78 (90%)	9 (10%)	7	24
13	K	90/99 (91%)	85 (94%)	5 (6%)	21	49
14	L	104/111 (94%)	98 (94%)	6 (6%)	20	48
15	M	100/101 (99%)	89 (89%)	11 (11%)	6	22
16	N	49/50 (98%)	44 (90%)	5 (10%)	7	24
17	O	79/80 (99%)	72 (91%)	7 (9%)	9	31
18	P	72/74 (97%)	68 (94%)	4 (6%)	21	49

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	Q	96/97 (99%)	88 (92%)	8 (8%)	11	35
20	R	64/77 (83%)	60 (94%)	4 (6%)	18	45
21	S	71/80 (89%)	67 (94%)	4 (6%)	21	49
22	T	75/82 (92%)	68 (91%)	7 (9%)	9	29
23	V	19/22 (86%)	18 (95%)	1 (5%)	22	51
All	All	1996/2112 (94%)	1822 (91%)	174 (9%)	10	33

5 of 174 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	H	26	VAL
11	I	79	LEU
20	R	54	ARG
10	H	83	ILE
11	I	5	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 60 such sidechains are listed below:

Mol	Chain	Res	Type
7	E	78	HIS
9	G	37	ASN
21	S	14	HIS
8	F	32	ASN
9	G	96	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1506/1522 (98%)	226 (15%)	73 (4%)
2	X	10/11 (90%)	0	0
3	W	3/4 (75%)	0	0
All	All	1519/1537 (98%)	226 (14%)	73 (4%)

5 of 226 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	8	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	9	G
1	A	31	G
1	A	32	A

5 of 73 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	560	U
1	A	913	A
1	A	1498	U
1	A	792	A
1	A	960	U

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 110 ligands modelled in this entry, 109 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	$\# Z > 2$
24	PAR	A	1545	-	45,45,45	1.55	8 (17%)	64,67,67	1.18	7 (10%)

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
24	PAR	A	1545	-	-	4/18/94/94	0/4/4/4

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1545	PAR	C64-C54	4.76	1.58	1.52
24	A	1545	PAR	O54-C14	3.63	1.51	1.41
24	A	1545	PAR	C11-C21	2.67	1.57	1.52
24	A	1545	PAR	O51-C11	2.61	1.48	1.41
24	A	1545	PAR	C31-C21	2.54	1.56	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1545	PAR	O54-C54-C64	3.52	112.56	106.01
24	A	1545	PAR	O33-C14-C24	3.37	114.02	108.22
24	A	1545	PAR	C14-O54-C54	2.93	119.44	113.69
24	A	1545	PAR	O52-C13-C23	2.91	113.99	107.96
24	A	1545	PAR	O52-C13-O43	-2.27	108.97	111.43

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	1545	PAR	C44-C54-C64-N64
24	A	1545	PAR	O54-C54-C64-N64
24	A	1545	PAR	C52-C42-O11-C11
24	A	1545	PAR	C23-C33-O33-C14

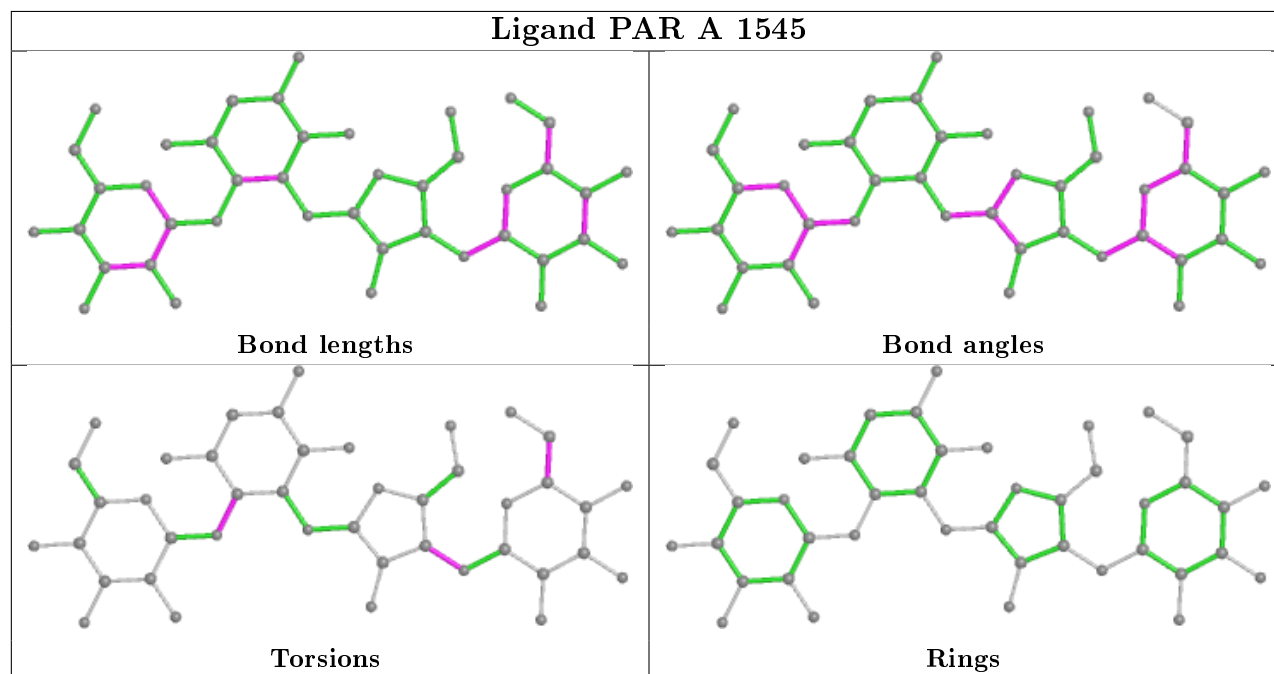
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	1545	PAR	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 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	A	1507/1522 (99%)	0.97	74 (4%) 29 13	31, 65, 156, 200	0
2	X	10/11 (90%)	0.22	0 100 100	79, 120, 147, 149	0
3	W	4/4 (100%)	0.73	0 100 100	63, 68, 79, 134	0
4	B	234/256 (91%)	0.29	6 (2%) 56 30	45, 102, 162, 200	0
5	C	206/239 (86%)	0.32	3 (1%) 73 51	44, 92, 150, 185	0
6	D	208/209 (99%)	0.49	11 (5%) 26 11	40, 73, 128, 164	0
7	E	150/162 (92%)	0.30	1 (0%) 87 72	35, 59, 110, 151	0
8	F	101/101 (100%)	0.10	0 100 100	54, 95, 138, 162	0
9	G	155/156 (99%)	0.21	4 (2%) 56 30	46, 80, 138, 172	0
10	H	138/138 (100%)	0.36	3 (2%) 62 38	32, 57, 101, 130	0
11	I	127/128 (99%)	0.69	8 (6%) 20 8	45, 93, 141, 168	0
12	J	98/105 (93%)	0.78	7 (7%) 16 6	49, 116, 172, 189	0
13	K	119/129 (92%)	0.54	3 (2%) 57 32	38, 67, 123, 173	0
14	L	124/135 (91%)	0.52	4 (3%) 47 24	30, 69, 120, 189	0
15	M	125/126 (99%)	0.84	14 (11%) 5 1	51, 85, 149, 181	0
16	N	60/61 (98%)	0.94	11 (18%) 1 0	53, 81, 126, 188	0
17	O	88/89 (98%)	0.34	1 (1%) 80 60	39, 72, 131, 191	0
18	P	83/88 (94%)	0.54	2 (2%) 59 34	37, 54, 89, 146	0
19	Q	104/105 (99%)	0.91	6 (5%) 23 9	33, 57, 124, 200	0
20	R	73/88 (82%)	0.37	3 (4%) 37 18	48, 79, 153, 193	0
21	S	80/93 (86%)	0.82	9 (11%) 5 1	65, 110, 155, 178	0
22	T	99/106 (93%)	0.41	1 (1%) 82 63	35, 61, 118, 160	0
23	V	24/27 (88%)	0.84	3 (12%) 3 1	45, 70, 135, 147	0
All	All	3917/4078 (96%)	0.67	174 (4%) 34 16	30, 73, 150, 200	0

The worst 5 of 174 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
19	Q	103	GLY	18.3
19	Q	102	GLY	13.3
15	M	126	LYS	13.1
15	M	124	PRO	12.7
19	Q	105	ALA	11.7

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(\AA^2)	Q<0.9
25	MG	X	502	1/1	0.19	1.74	67,67,67,67	1
25	MG	A	1607	1/1	0.33	0.34	67,67,67,67	1
25	MG	A	1575	1/1	0.38	0.54	67,67,67,67	1
25	MG	A	1594	1/1	0.58	1.02	67,67,67,67	1
25	MG	A	1630	1/1	0.66	0.33	67,67,67,67	0
25	MG	A	1621	1/1	0.67	0.32	67,67,67,67	0
25	MG	A	1565	1/1	0.69	0.32	67,67,67,67	0
25	MG	A	1598	1/1	0.72	0.16	67,67,67,67	0
25	MG	A	467	1/1	0.72	0.79	67,67,67,67	0
25	MG	A	1573	1/1	0.72	0.37	67,67,67,67	0
25	MG	A	1562	1/1	0.73	0.26	67,67,67,67	0
25	MG	A	441	1/1	0.74	0.26	67,67,67,67	0
25	MG	A	470	1/1	0.74	0.26	67,67,67,67	0
25	MG	A	1568	1/1	0.76	0.31	67,67,67,67	0
25	MG	A	1586	1/1	0.76	0.33	67,67,67,67	0
25	MG	A	1613	1/1	0.76	0.31	67,67,67,67	0
25	MG	A	1592	1/1	0.77	0.38	67,67,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
25	MG	A	214	1/1	0.78	0.16	67,67,67,67	0
25	MG	A	1571	1/1	0.79	0.31	67,67,67,67	0
25	MG	A	1585	1/1	0.80	0.30	67,67,67,67	0
25	MG	A	1601	1/1	0.80	0.14	67,67,67,67	0
25	MG	J	449	1/1	0.80	0.30	67,67,67,67	0
25	MG	A	466	1/1	0.80	0.23	67,67,67,67	0
25	MG	A	210	1/1	0.80	0.15	67,67,67,67	0
25	MG	A	1627	1/1	0.81	0.28	67,67,67,67	0
25	MG	A	1633	1/1	0.81	0.19	67,67,67,67	0
25	MG	A	1628	1/1	0.82	0.28	67,67,67,67	0
25	MG	A	1603	1/1	0.83	0.24	67,67,67,67	0
25	MG	A	1634	1/1	0.83	0.33	67,67,67,67	0
25	MG	A	211	1/1	0.84	0.33	67,67,67,67	0
25	MG	A	1619	1/1	0.84	0.17	67,67,67,67	0
25	MG	A	1616	1/1	0.84	0.27	67,67,67,67	0
25	MG	A	1597	1/1	0.84	0.11	67,67,67,67	0
25	MG	A	87	1/1	0.85	0.34	67,67,67,67	0
25	MG	A	1583	1/1	0.85	0.34	67,67,67,67	0
25	MG	A	1610	1/1	0.85	0.54	67,67,67,67	1
25	MG	A	493	1/1	0.85	0.30	67,67,67,67	1
25	MG	A	1632	1/1	0.86	0.28	67,67,67,67	0
25	MG	A	1626	1/1	0.86	0.12	67,67,67,67	0
25	MG	A	1620	1/1	0.86	0.19	67,67,67,67	0
25	MG	A	86	1/1	0.86	0.32	67,67,67,67	0
25	MG	A	1590	1/1	0.87	0.35	67,67,67,67	0
25	MG	A	1574	1/1	0.87	0.39	67,67,67,67	0
25	MG	A	1608	1/1	0.88	0.29	67,67,67,67	0
25	MG	A	1577	1/1	0.88	0.31	67,67,67,67	0
25	MG	A	1576	1/1	0.88	0.43	67,67,67,67	0
25	MG	A	1548	1/1	0.88	0.25	67,67,67,67	0
25	MG	A	1602	1/1	0.88	0.23	67,67,67,67	0
25	MG	A	471	1/1	0.88	0.23	67,67,67,67	0
25	MG	A	1559	1/1	0.89	0.55	67,67,67,67	0
25	MG	A	1604	1/1	0.89	0.37	67,67,67,67	0
25	MG	A	1605	1/1	0.89	0.27	67,67,67,67	0
25	MG	A	1622	1/1	0.89	0.38	67,67,67,67	0
25	MG	A	1558	1/1	0.89	0.33	67,67,67,67	0
25	MG	A	1617	1/1	0.89	0.25	67,67,67,67	0
25	MG	A	1611	1/1	0.89	0.24	67,67,67,67	0
25	MG	A	1624	1/1	0.89	0.35	67,67,67,67	0
25	MG	A	1566	1/1	0.90	0.41	67,67,67,67	0
25	MG	A	1587	1/1	0.90	0.42	67,67,67,67	0

Continued on next page...

Continued from previous page...

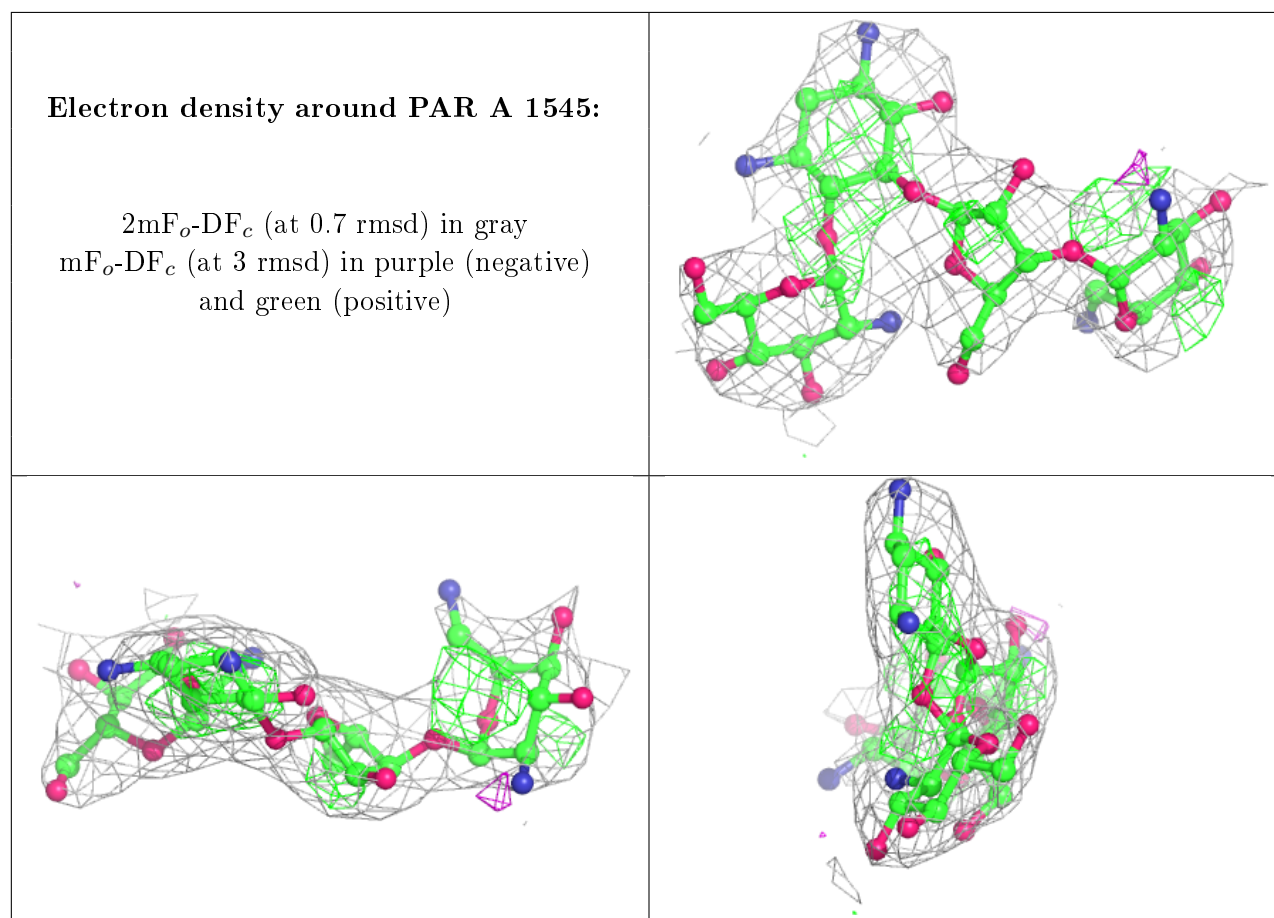
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
25	MG	A	1600	1/1	0.90	0.23	67,67,67,67	0
25	MG	X	500	1/1	0.90	0.86	67,67,67,67	1
25	MG	A	1581	1/1	0.90	0.47	67,67,67,67	0
25	MG	A	1615	1/1	0.90	0.25	67,67,67,67	0
25	MG	A	1547	1/1	0.90	0.40	67,67,67,67	0
25	MG	A	1570	1/1	0.91	0.40	67,67,67,67	0
25	MG	A	1623	1/1	0.91	0.17	67,67,67,67	0
25	MG	A	1572	1/1	0.91	0.24	67,67,67,67	0
25	MG	A	1561	1/1	0.91	0.21	67,67,67,67	0
25	MG	A	1606	1/1	0.91	0.35	67,67,67,67	0
25	MG	A	1629	1/1	0.91	0.33	67,67,67,67	0
25	MG	A	1555	1/1	0.91	0.41	67,67,67,67	0
25	MG	A	1567	1/1	0.92	0.42	67,67,67,67	0
25	MG	A	1595	1/1	0.92	0.14	67,67,67,67	0
25	MG	A	1596	1/1	0.92	0.29	67,67,67,67	0
25	MG	A	1582	1/1	0.92	0.27	67,67,67,67	0
24	PAR	A	1545	42/42	0.92	0.34	67,67,67,67	0
25	MG	A	1578	1/1	0.93	0.29	67,67,67,67	0
25	MG	A	1584	1/1	0.93	0.34	67,67,67,67	0
25	MG	A	1564	1/1	0.93	0.48	67,67,67,67	0
25	MG	A	1609	1/1	0.93	0.30	67,67,67,67	0
25	MG	A	71	1/1	0.93	0.39	67,67,67,67	0
25	MG	A	1614	1/1	0.94	0.16	67,67,67,67	0
25	MG	A	1550	1/1	0.94	0.35	67,67,67,67	0
25	MG	A	1549	1/1	0.94	0.48	67,67,67,67	0
25	MG	A	1554	1/1	0.94	0.33	67,67,67,67	0
25	MG	A	1560	1/1	0.95	0.46	67,67,67,67	0
25	MG	A	1612	1/1	0.95	0.33	67,67,67,67	0
25	MG	A	1557	1/1	0.95	0.40	67,67,67,67	0
25	MG	A	1569	1/1	0.95	0.40	67,67,67,67	0
25	MG	A	1553	1/1	0.95	0.51	67,67,67,67	0
25	MG	A	1618	1/1	0.95	0.33	67,67,67,67	0
25	MG	A	1593	1/1	0.95	0.33	67,67,67,67	0
25	MG	A	469	1/1	0.95	0.13	67,67,67,67	1
25	MG	A	1556	1/1	0.96	0.53	67,67,67,67	0
25	MG	A	1579	1/1	0.96	0.32	67,67,67,67	0
25	MG	A	1625	1/1	0.96	0.17	67,67,67,67	0
25	MG	A	1552	1/1	0.96	0.47	67,67,67,67	0
25	MG	A	1635	1/1	0.96	0.26	67,67,67,67	1
25	MG	A	1546	1/1	0.96	0.33	67,67,67,67	0
25	MG	A	1591	1/1	0.96	0.22	67,67,67,67	0
25	MG	A	1563	1/1	0.97	0.36	67,67,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
25	MG	A	1580	1/1	0.97	0.33	67,67,67,67	0
25	MG	A	1589	1/1	0.97	0.51	67,67,67,67	0
25	MG	A	1631	1/1	0.97	0.08	67,67,67,67	0
25	MG	A	1588	1/1	0.97	0.47	67,67,67,67	0
25	MG	A	1551	1/1	0.97	0.47	67,67,67,67	0
25	MG	A	1599	1/1	0.97	0.24	67,67,67,67	0
25	MG	A	473	1/1	0.99	0.09	67,67,67,67	1
26	ZN	D	306	1/1	0.99	0.43	67,67,67,67	0
26	ZN	N	307	1/1	0.99	0.23	67,67,67,67	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.