



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 06:08 PM UTC

PDB ID : 1XMO / pdb_00001xmo
Title : Crystal Structure of mnm5U34t6A37-tRNA^{Lys}UUU Complexed with AAG-mRNA in the Decoding Center
Authors : Murphy, F.V.; Ramakrishnan, V.; Malkiewicz, A.; Agris, P.F.
Deposited on : 2004-10-04
Resolution : 3.25 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

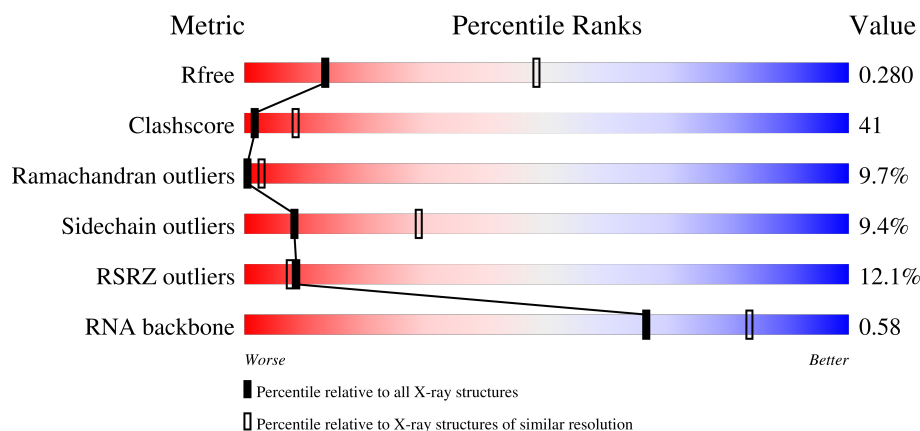
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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}	180053	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (3.30-3.22)
RNA backbone	3983	1006 (3.54-2.98)

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	A	1522	12% 27% 55% 13% . .
2	W	3	100%
3	X	11	45% 36% 55% 9%
4	B	256	14% 13% 62% 14% . 9%

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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	1562	-	-	-	X
25	MG	A	1615	-	-	-	X
25	MG	A	214	-	-	-	X
3	T6A	X	37	X	-	-	-

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 52063 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 A-Site Messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	W	3	Total	C	N	O	P	0	0	0
			64	30	15	17	2			

- Molecule 3 is a RNA chain called Anticodon Transfer RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	X	11	Total	C	N	O	P	0	0	0
			239	110	38	81	10			

- Molecule 4 is a protein called 30S 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 30S 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 30S 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 30S 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 30S 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 30S 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 30S 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 30S ribosomal protein S9.

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

- Molecule 12 is a protein called 30S 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 30S 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 30S 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 30S 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 30S 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 30S 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 30S 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 30S 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 30S 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 30S 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			

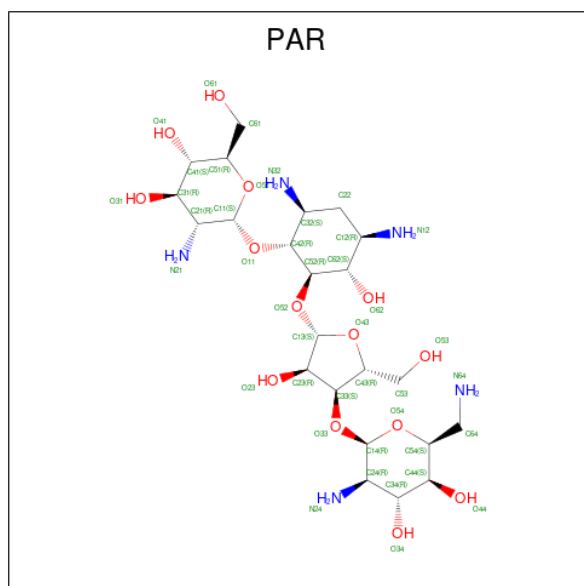
- Molecule 22 is a protein called 30S ribosomal protein S20.

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 30S 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 (CCD ID: 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 (CCD ID: MG) (formula: Mg).

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	X	2	Total 2	Mg 2	0	0
25	J	1	Total 1	Mg 1	0	0

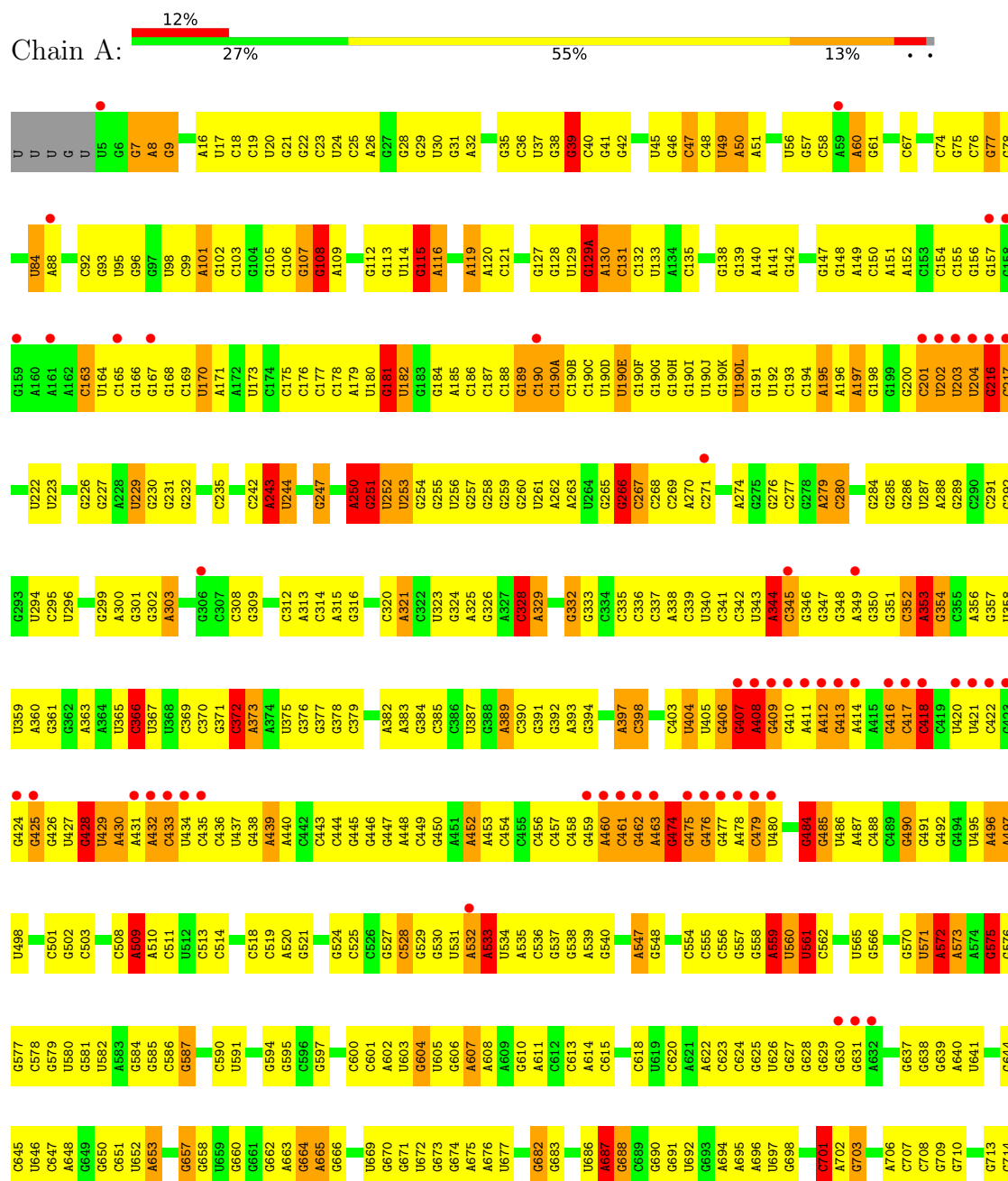
- Molecule 26 is ZINC ION (CCD ID: ZN) (formula: Zn).

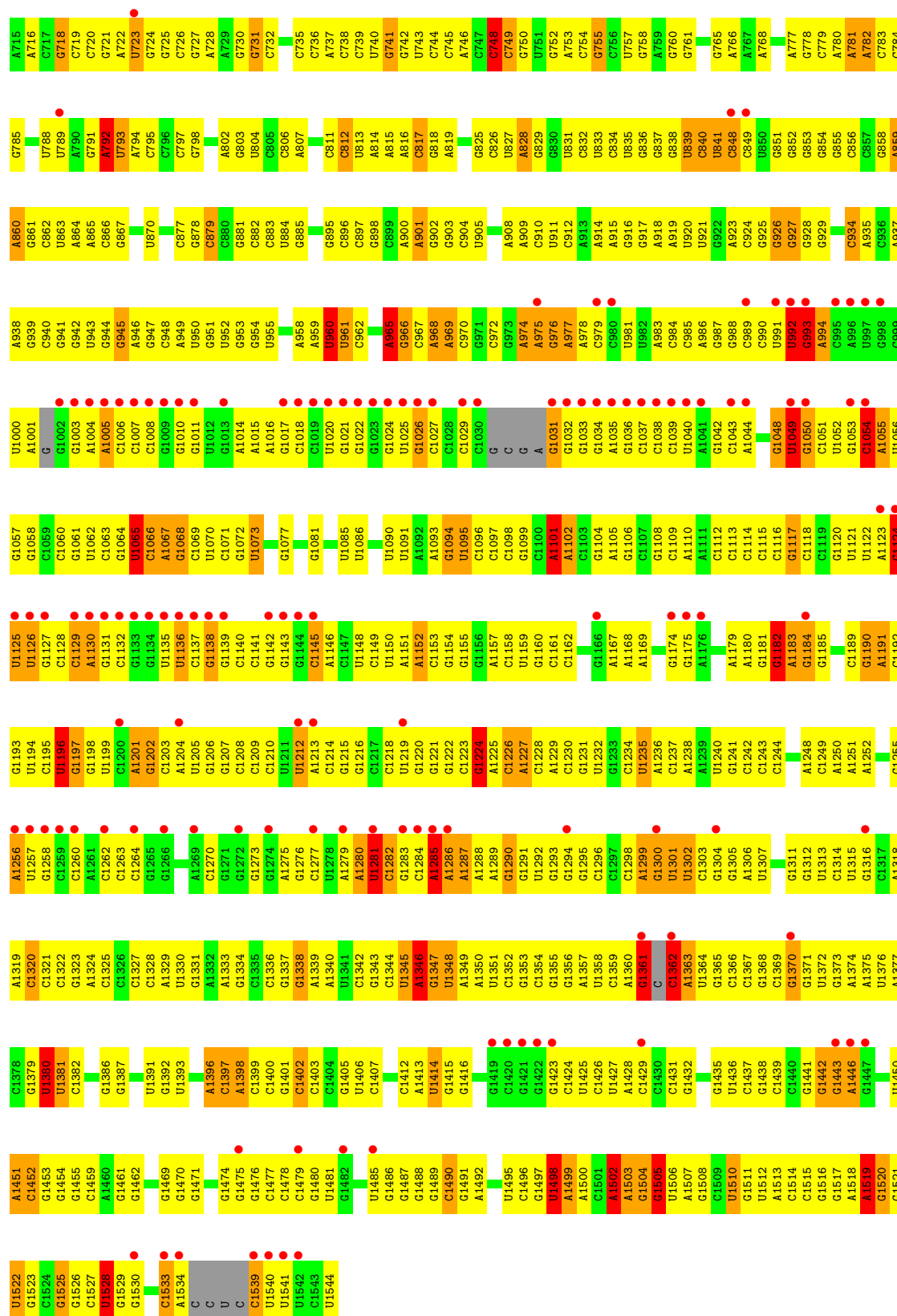
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
26	D	1	Total 1	Zn 1	0	0
26	N	1	Total 1	Zn 1	0	0

3 Residue-property plots [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

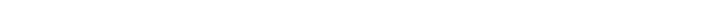




Chain W: 100%

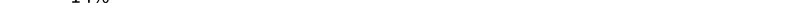
A1
A2
G3

- Molecule 3: Anticodon Transfer RNA

Chain X: 

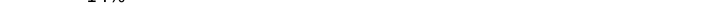
G30	A31	C32	U33	U34	U35	U36	A37	A38	U39	C40
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Molecule 4: 30S ribosomal protein S2

Chain B:  14% 13% 62% 14% 9%

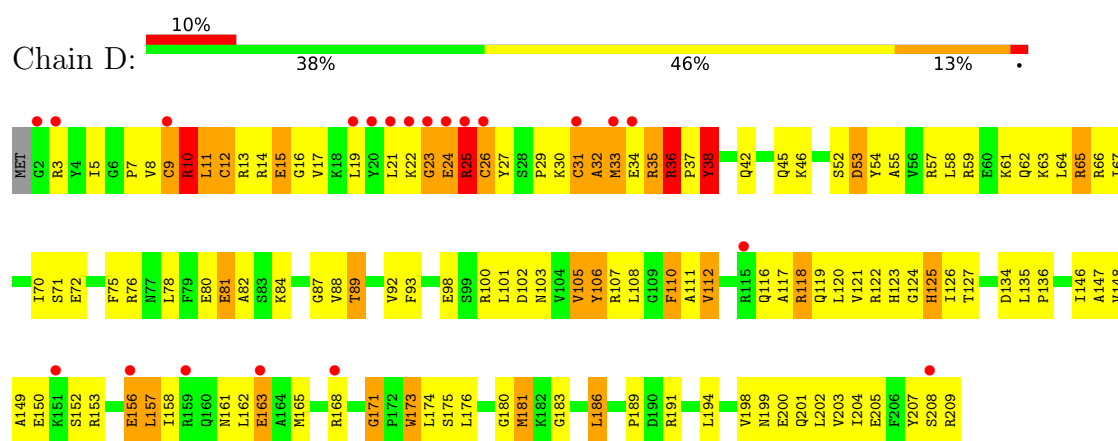
ALA	THR	F181	L121	L61	MET
	GLU	P183	F122	A62	PRO
	THR	T184	A123	M63	VAL
	PRO	I186	S124	R64	GLU
	GLU	A186	P125	G65	ILE
	GLY	L187	E126	G66	THR
	GLU		I127	T67	V7
	SER	T190	E128	I68	K8
	GLU	D191	E129	L69	E9
	VAL	S192	P131	V71	L10
ALA	GLU	D193	K132	G72	E12
	GLU	P194	K133	T73	A13
	GLU	D195	E134	K74	G14
	GLU	L196	Q135	K75	V15
	GLU	V197	V136	Q76	H16
	GLU	D198	R137	A77	F17
	GLU	T199	L138	F78	G18
	GLU	I200	K139	D79	H19
	GLU	I201	H140	E80	E20
	GLU	P202	E141	V81	R21
ALA	GLU	G203	L142	R82	K22
	GLU	N204	E143	M83	R23
	GLU	D205	R144	E84	W24
	GLU	D206	L145	A85	N25
	GLU	A207	Q146	E86	P26
	GLU	I208	K147	R87	K27
	GLU	R209	Y148	A88	F28
	GLU	S210	L149	G89	A29
	GLU	T211	S150	M90	R30
	GLU	Q212	G151	P91	Y31
ALA	GLU	L213	F152	Y92	I32
	GLU	I214	R153	V93	Y33
	GLU	L215	L154	N94	A34
	GLU	S216	L155	Q95	E35
	GLU	R217	K156	R96	R36
	GLU	A218	L157	W97	N37
	GLU	V219	L158	L98	G38
	GLU	D220	P159	G99	I39
	GLU	L221	D160	G100	H40
	GLU	L222	A161	M101	I41
ALA	GLU	T223	L162	L102	I42
	GLU	Q224	F163	T103	D43
	GLU	A225	V164	N104	L44
	GLU	R226	V165	F105	Q45
	GLU		D166	K106	K46
	GLU	V229	P167	T107	T47
	GLU	V230	T168	I108	M48
	GLU	E231	K169	S109	E49
	GLU	P232	Q110	P110	E50
	GLU	S233	A171	R111	L51
ALA	GLU	P234	I172	V112	E52
	GLU		A173	H113	R53
	GLU	A237	V174	R114	T54
	GLU	L238	R175	L115	F55
	GLU	V239	E176	E116	R56
	GLU	Q240	A177	E117	F57
	GLU		R178	L118	I58
	GLU	ALA	K179	E119	E59
	GLU		L180	A120	D60

- Molecule 5: 30S ribosomal protein S3

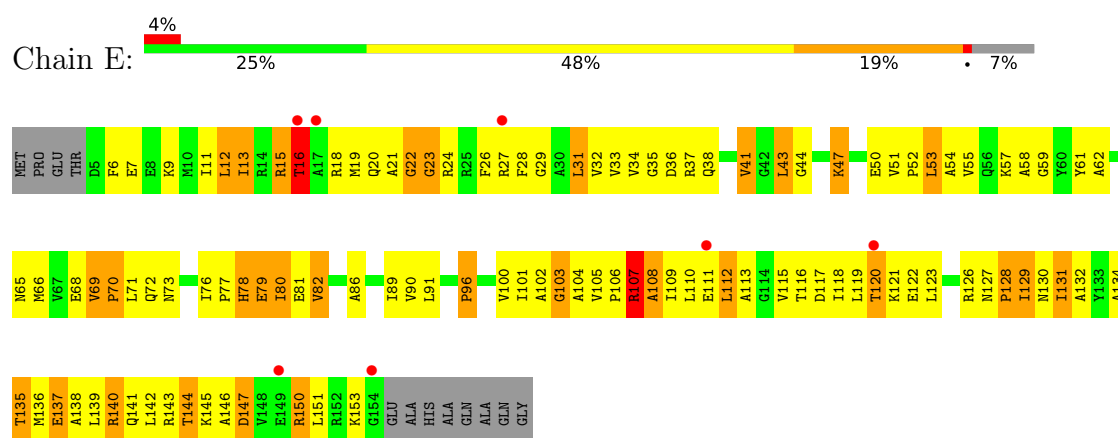
Chain C:  14% 20% 48% 18% 14%

Y193	E125	M63	MET
G194	R126	V64	G2
V195	R127	A65	N3
L196	F128	V66	K4
	A129	T67	I5
K199		V68	H6
A200	R132	H69	P7
A201	A133	V70	I8
I202	I134		G9
F203	K135	F73	F10
L204	Q136	G74	R11
G205	A137	V75	L12
E206	V138	W76	G13
V207	Q139	I77	I14
ILE	R140	G78	T15
GLY	V141	R79	R16
GLY	M142	G80	D17
GLN	E143	G81	K18
LYS	S144	E82	E19
PRO	G145	R83	S20
LYS	A146	R84	R21
ALA	K147	R85	W22
ARG	G148	V86	Y23
PRO	A149	L87	A24
GLU	K150	R88	G25
LEU	V151	E89	K26
PRO	I152	E90	K27
LYS	V153	L91	Q28
ALA	S154	A92	Y29
GLU	G155	K93	R30
ARG	R156	L94	H31
GLU	I157	T95	L32
PRO		G96	L33
ARG	A160	K97	L34
ARG	F161	N98	E35
ARG	Q162	V99	D36
ARG	A163	A100	Q37
PRO	R164	L101	R38
ALA	T165	M102	I39
VAL	E166		R40
ARG	V167	E105	
VAL	A168	V106	L43
LYS	A169	Q107	E44
LYS	Q170	M108	K45
GLU	G171	P109	E46
GLU	R172	M110	L47
		L111	Y48
		S112	S49
		A113	A50
		P114	G51
		L115	L52
		V116	A53
		A117	
		Q118	D56
		R119	I57
		V120	E58
		A121	R59
		E122	A60
		Q123	A61
		T124	R62

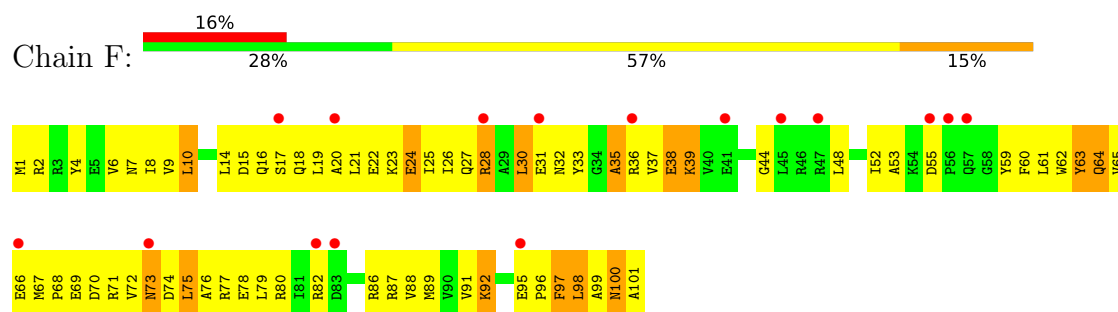
- Molecule 6: 30S ribosomal protein S4



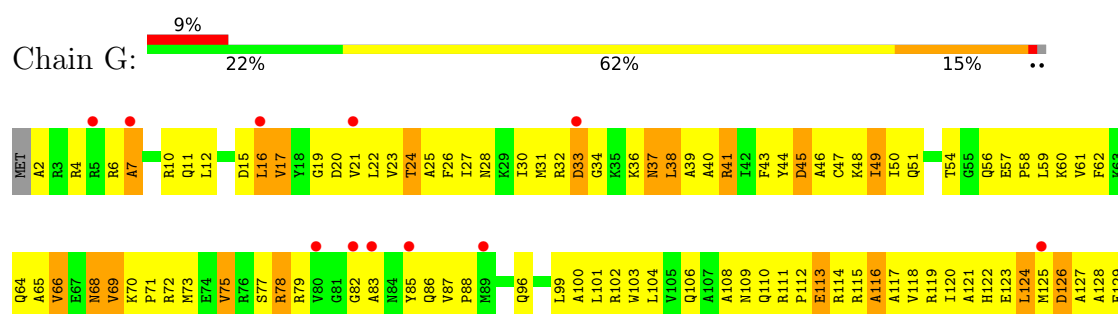
• Molecule 7: 30S ribosomal protein S5



• Molecule 8: 30S ribosomal protein S6

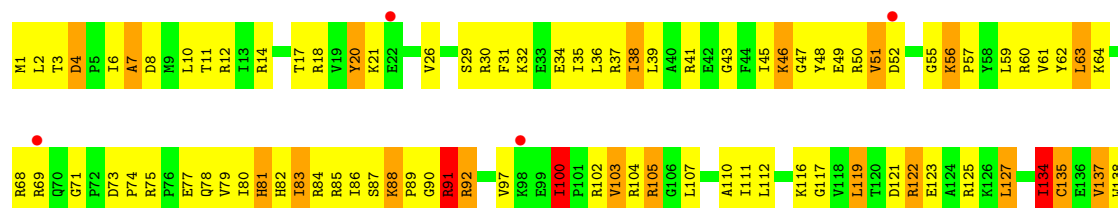


• Molecule 9: 30S ribosomal protein S7

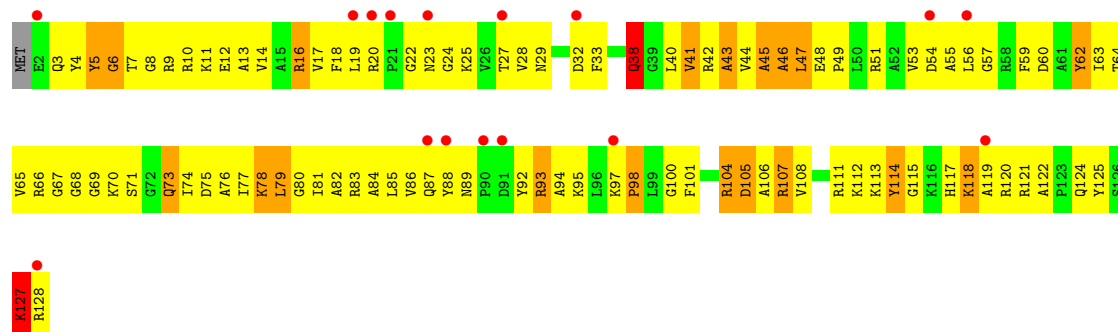




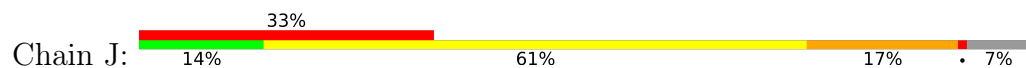
- Molecule 10: 30S ribosomal protein S8



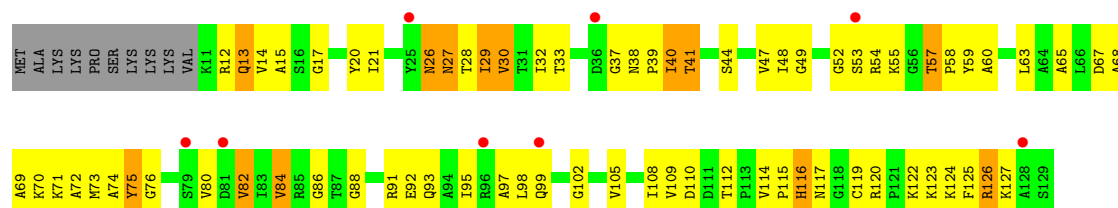
- Molecule 11: 30S ribosomal protein S9



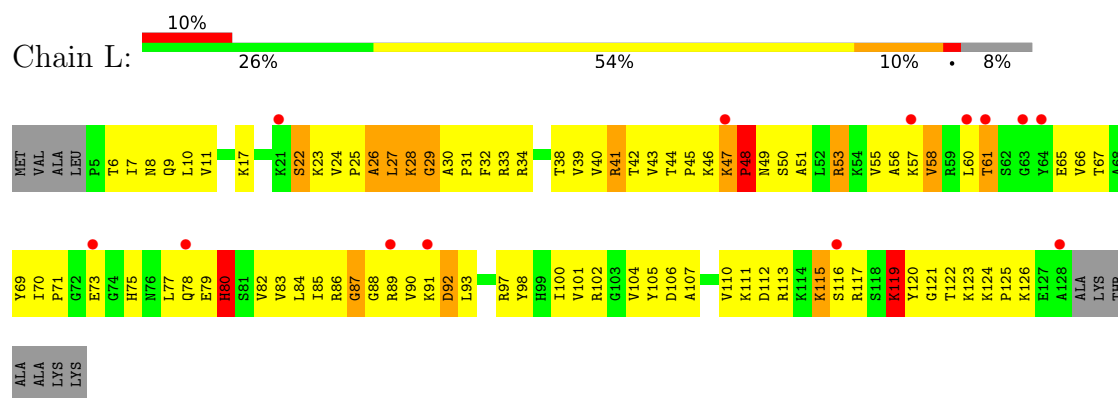
- Molecule 12: 30S ribosomal protein S10



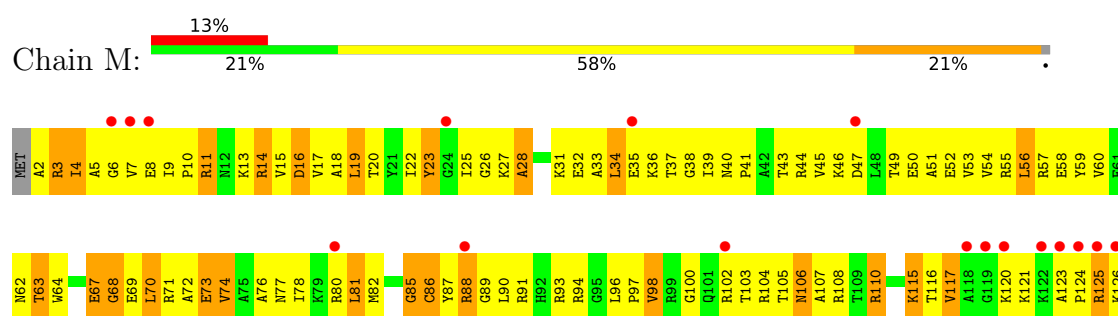
- Molecule 13: 30S ribosomal protein S11



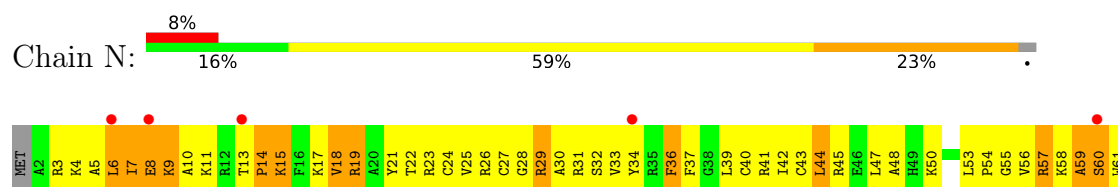
- Molecule 14: 30S ribosomal protein S12



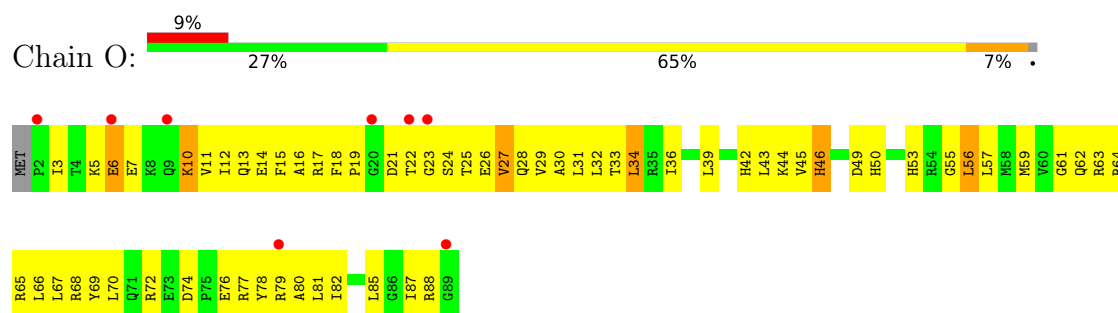
- Molecule 15: 30S ribosomal protein S13



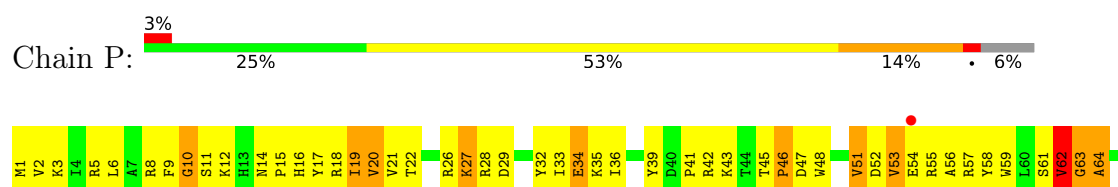
- Molecule 16: 30S ribosomal protein S14



- Molecule 17: 30S ribosomal protein S15

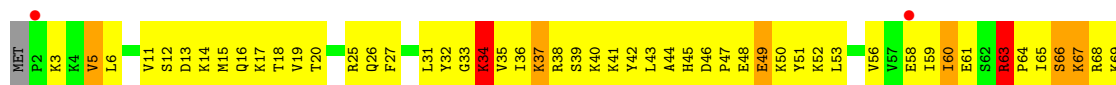


- Molecule 18: 30S ribosomal protein S16

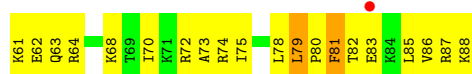
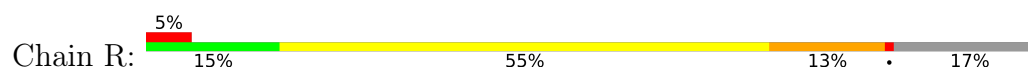




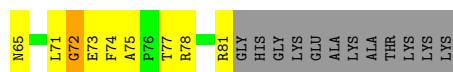
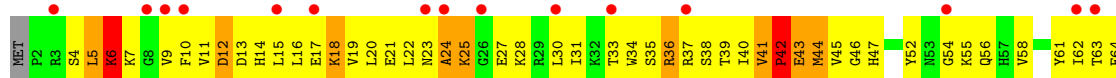
- Molecule 19: 30S ribosomal protein S17



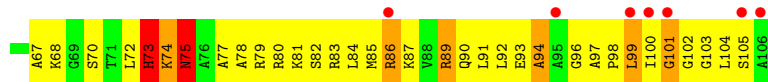
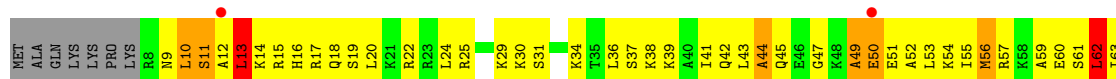
- Molecule 20: 30S ribosomal protein S18



- Molecule 21: 30S ribosomal protein S19

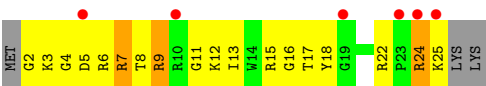


- Molecule 22: 30S ribosomal protein S20



- Molecule 23: 30S ribosomal protein Thx





4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	400.81Å 400.81Å 176.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	99.00 – 3.25 99.00 – 3.25	Depositor EDS
% Data completeness (in resolution range)	5.0 (99.00-3.25) 89.2 (99.00-3.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 3.26Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.231 , 0.284 0.228 , 0.280	Depositor DCC
R_{free} test set	10562 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	85.2	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.45 , 300.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	52063	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 2.22% 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: MNU, PAR, ZN, T6A, MG

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	0.47	2/36244 (0.0%)	0.72	65/56567 (0.1%)
2	W	0.53	0/72	1.11	2/111 (1.8%)
3	X	0.52	0/203	0.73	0/311
4	B	0.41	0/1935	1.01	14/2609 (0.5%)
5	C	0.43	0/1636	0.94	3/2205 (0.1%)
6	D	0.51	0/1733	1.02	12/2318 (0.5%)
7	E	0.55	0/1162	1.12	6/1564 (0.4%)
8	F	0.38	0/856	0.86	1/1154 (0.1%)
9	G	0.45	0/1276	0.99	9/1709 (0.5%)
10	H	0.58	0/1136	1.20	14/1527 (0.9%)
11	I	0.41	0/1029	0.97	5/1378 (0.4%)
12	J	0.40	0/805	1.07	4/1082 (0.4%)
13	K	0.57	0/900	1.05	6/1213 (0.5%)
14	L	0.57	0/986	1.20	5/1320 (0.4%)
15	M	0.45	0/1008	1.00	3/1347 (0.2%)
16	N	0.46	0/501	1.09	3/664 (0.5%)
17	O	0.47	0/745	0.88	2/992 (0.2%)
18	P	0.57	0/716	1.13	6/963 (0.6%)
19	Q	0.56	0/870	1.14	6/1159 (0.5%)
20	R	0.42	0/603	1.04	5/799 (0.6%)
21	S	0.38	0/661	1.01	3/890 (0.3%)
22	T	0.56	0/764	1.15	6/1006 (0.6%)
23	V	0.52	0/212	1.06	1/277 (0.4%)
All	All	0.47	2/56053 (0.0%)	0.84	181/83165 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	4	60
3	X	1	0
All	All	5	60

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1361	G	O5'-C5'	6.30	1.51	1.42
1	A	1362	C	O5'-C5'	5.90	1.51	1.42

The worst 5 of 181 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	575	G	C2'-C3'-O3'	14.16	130.74	109.50
14	L	26	ALA	N-CA-C	-13.98	98.15	112.97
1	A	115	G	C2'-C3'-O3'	13.96	130.44	109.50
1	A	559	A	C2'-C3'-O3'	13.74	130.12	109.50
1	A	243	A	C2'-C3'-O3'	13.67	130.01	109.50

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	181	G	C3'
1	A	243	A	C3'
1	A	559	A	C3'
1	A	1528	U	C3'
3	X	37	T6A	C14

5 of 60 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	G	Sidechain
1	A	108	G	Sidechain
1	A	39	G	Sidechain
1	A	77	G	Sidechain
1	A	84	U	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	1334	0
2	W	64	0	35	4	0
3	X	239	0	127	7	0
4	B	1900	0	1951	329	0
5	C	1612	0	1677	257	0
6	D	1703	0	1764	165	0
7	E	1146	0	1207	143	0
8	F	843	0	857	110	0
9	G	1257	0	1296	147	0
10	H	1116	0	1177	120	0
11	I	1011	0	1043	158	0
12	J	792	0	835	129	0
13	K	885	0	904	74	0
14	L	970	0	1057	132	0
15	M	997	0	1072	160	0
16	N	492	0	530	74	0
17	O	734	0	771	85	0
18	P	700	0	720	90	0
19	Q	857	0	930	129	0
20	R	597	0	668	106	0
21	S	647	0	673	86	0
22	T	762	0	856	98	0
23	V	208	0	221	21	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	1	0
All	All	52063	0	36762	3649	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 41.

The worst 5 of 3649 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:1489:G:H2'	1:A:1490:C:H5''	1.26	1.10
6:D:36:ARG:H	6:D:37:PRO:HD3	1.13	1.08
5:C:26:LYS:H	5:C:26:LYS:HD3	1.14	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:179:ARG:HG2	5:C:180:ALA:H	0.98	1.06
4:B:132:LYS:HA	4:B:135:GLN:HB3	1.36	1.05

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	
4	B	232/256 (91%)	129 (56%)	80 (34%)	23 (10%)	0	3
5	C	204/239 (85%)	123 (60%)	48 (24%)	33 (16%)	0	1
6	D	206/209 (99%)	151 (73%)	38 (18%)	17 (8%)	0	4
7	E	148/162 (91%)	120 (81%)	18 (12%)	10 (7%)	1	6
8	F	99/101 (98%)	68 (69%)	24 (24%)	7 (7%)	1	6
9	G	153/156 (98%)	99 (65%)	41 (27%)	13 (8%)	0	4
10	H	136/138 (99%)	106 (78%)	25 (18%)	5 (4%)	2	15
11	I	125/128 (98%)	85 (68%)	27 (22%)	13 (10%)	0	2
12	J	96/105 (91%)	57 (59%)	23 (24%)	16 (17%)	0	1
13	K	117/129 (91%)	85 (73%)	26 (22%)	6 (5%)	1	10
14	L	122/135 (90%)	85 (70%)	24 (20%)	13 (11%)	0	2
15	M	123/126 (98%)	75 (61%)	30 (24%)	18 (15%)	0	1
16	N	58/61 (95%)	34 (59%)	16 (28%)	8 (14%)	0	1
17	O	86/89 (97%)	54 (63%)	28 (33%)	4 (5%)	2	11
18	P	81/88 (92%)	59 (73%)	16 (20%)	6 (7%)	1	5
19	Q	102/105 (97%)	75 (74%)	17 (17%)	10 (10%)	0	3
20	R	71/88 (81%)	50 (70%)	16 (22%)	5 (7%)	1	6
21	S	78/93 (84%)	56 (72%)	14 (18%)	8 (10%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	T	97/106 (92%)	56 (58%)	30 (31%)	11 (11%)	0	2
23	V	22/27 (82%)	18 (82%)	2 (9%)	2 (9%)	0	3
All	All	2356/2541 (93%)	1585 (67%)	543 (23%)	228 (10%)	0	3

5 of 228 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	B	13	ALA
4	B	15	VAL
4	B	16	HIS
4	B	21	ARG
4	B	24	TRP

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%)	183 (91%)	19 (9%)	8	29
5	C	160/188 (85%)	145 (91%)	15 (9%)	8	29
6	D	180/181 (99%)	161 (89%)	19 (11%)	6	24
7	E	115/123 (94%)	90 (78%)	25 (22%)	1	4
8	F	90/90 (100%)	82 (91%)	8 (9%)	9	30
9	G	126/127 (99%)	115 (91%)	11 (9%)	9	31
10	H	119/119 (100%)	104 (87%)	15 (13%)	4	19
11	I	98/99 (99%)	89 (91%)	9 (9%)	8	29
12	J	87/92 (95%)	84 (97%)	3 (3%)	32	57
13	K	90/99 (91%)	79 (88%)	11 (12%)	5	20
14	L	104/111 (94%)	99 (95%)	5 (5%)	23	50
15	M	100/101 (99%)	90 (90%)	10 (10%)	7	26
16	N	49/50 (98%)	46 (94%)	3 (6%)	17	44
17	O	79/80 (99%)	75 (95%)	4 (5%)	21	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	P	72/74 (97%)	66 (92%)	6 (8%)	10	34
19	Q	96/97 (99%)	88 (92%)	8 (8%)	10	34
20	R	64/77 (83%)	60 (94%)	4 (6%)	16	43
21	S	71/80 (89%)	66 (93%)	5 (7%)	14	40
22	T	75/82 (92%)	68 (91%)	7 (9%)	8	29
23	V	19/22 (86%)	19 (100%)	0	100	100
All	All	1996/2112 (94%)	1809 (91%)	187 (9%)	8	29

5 of 187 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	I	78	LYS
15	M	70	LEU
11	I	118	LYS
13	K	44	SER
16	N	7	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 71 such sidechains are listed below:

Mol	Chain	Res	Type
15	M	101	GLN
17	O	37	ASN
21	S	23	ASN
7	E	65	ASN
6	D	201	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1506/1522 (98%)	241 (16%)	62 (4%)
2	W	2/3 (66%)	1 (50%)	0
3	X	10/11 (90%)	0	0
All	All	1518/1536 (98%)	242 (15%)	62 (4%)

5 of 242 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	8	A

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Mol	Chain	Res	Type
1	A	9	G
1	A	31	G
1	A	32	A
1	A	39	G

5 of 62 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	701	C
1	A	1397	C
1	A	975	A
1	A	1380	U
1	A	1504	G

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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
3	T6A	X	37	3	31,34,35	1.34	6 (19%)	43,49,52	3.15	10 (23%)
3	MNU	X	34	3,2	21,24,25	0.55	0	27,34,37	0.46	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	T6A	X	37	3	1/1/9/11	4/23/41/42	0/3/3/3
3	MNU	X	34	3,2	-	3/10/28/29	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	37	T6A	O14-C14	-3.12	1.34	1.43
3	X	37	T6A	ODA-C13	3.07	1.31	1.22
3	X	37	T6A	C15-C14	-2.87	1.43	1.51
3	X	37	T6A	ODB-C13	-2.79	1.21	1.30
3	X	37	T6A	C12-N11	-2.45	1.40	1.45

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	X	37	T6A	O14-C14-C15	11.89	145.26	109.68
3	X	37	T6A	ODA-C13-C12	-6.90	98.94	121.86
3	X	37	T6A	O14-C14-C12	-6.88	95.20	109.07
3	X	37	T6A	N6-C10-N11	6.55	122.78	113.77
3	X	37	T6A	C12-N11-C10	6.42	132.66	121.99

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	X	37	T6A	C14

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	X	34	MNU	C4-C5-C7-N8
3	X	37	T6A	C13-C12-C14-O14
3	X	37	T6A	N11-C12-C14-O14
3	X	37	T6A	C3'-C4'-C5'-O5'
3	X	34	MNU	C6-C5-C7-N8

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	X	37	T6A	2	0
3	X	34	MNU	3	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	-	44,45,45	1.63	10 (22%)	63,67,67	1.11	4 (6%)

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 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1545	PAR	O54-C14	4.02	1.52	1.41
24	A	1545	PAR	C31-C21	3.66	1.58	1.53
24	A	1545	PAR	O51-C11	2.94	1.49	1.41
24	A	1545	PAR	O33-C14	2.85	1.49	1.41
24	A	1545	PAR	O33-C33	2.82	1.51	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1545	PAR	O52-C13-O43	-3.40	107.89	111.37
24	A	1545	PAR	O54-C54-C64	3.34	112.49	106.07
24	A	1545	PAR	O33-C14-C24	3.21	113.33	108.08
24	A	1545	PAR	C14-O54-C54	3.13	119.83	113.72

There are no chirality outliers.

All (4) torsion outliers are listed below:

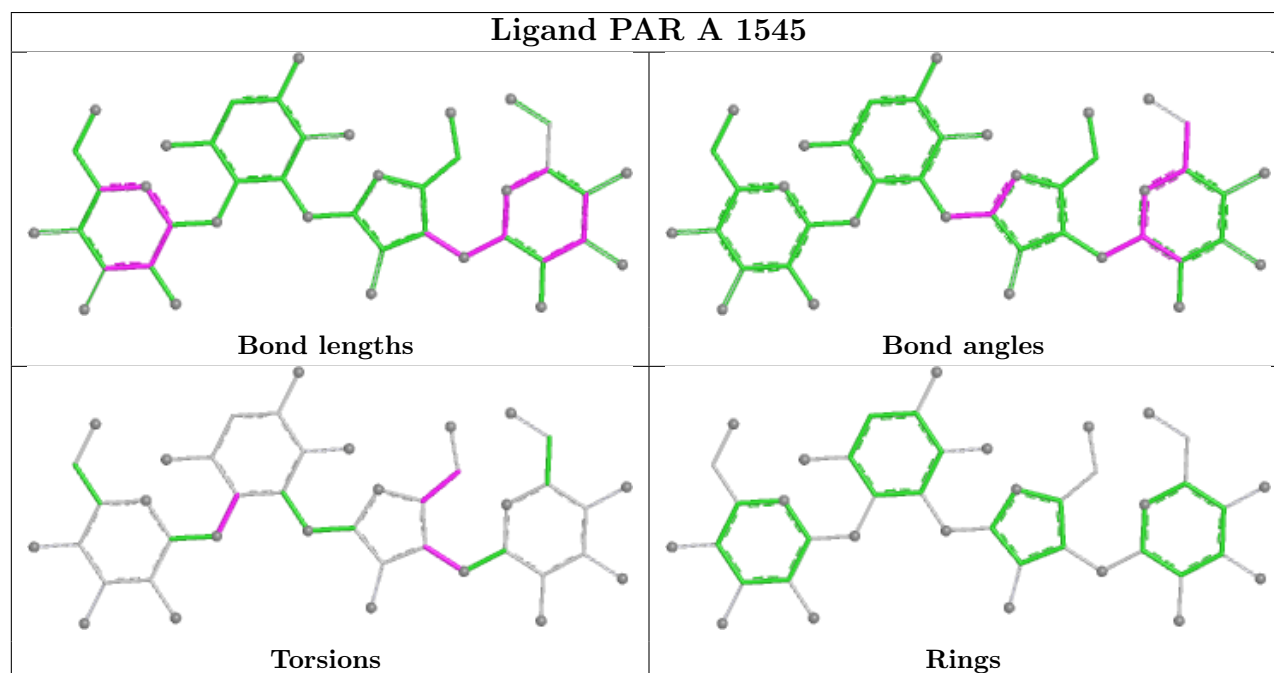
Mol	Chain	Res	Type	Atoms
24	A	1545	PAR	O43-C43-C53-O53
24	A	1545	PAR	C52-C42-O11-C11
24	A	1545	PAR	C23-C33-O33-C14
24	A	1545	PAR	C33-C43-C53-O53

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%)	0.77	188 (12%) 8 7	30, 65, 160, 200	0
2	W	3/3 (100%)	0.37	0 100 100	56, 56, 63, 72	0
3	X	9/11 (81%)	1.94	5 (55%) 0 0	64, 101, 157, 157	0
4	B	234/256 (91%)	0.90	36 (15%) 5 5	37, 100, 173, 200	0
5	C	206/239 (86%)	0.94	34 (16%) 4 4	44, 93, 169, 200	0
6	D	208/209 (99%)	0.62	21 (10%) 12 10	33, 71, 149, 200	0
7	E	150/162 (92%)	0.36	7 (4%) 36 24	27, 63, 122, 200	0
8	F	101/101 (100%)	0.92	16 (15%) 5 4	48, 103, 154, 174	0
9	G	155/156 (99%)	0.63	14 (9%) 15 12	41, 81, 152, 200	0
10	H	138/138 (100%)	0.28	4 (2%) 53 36	20, 54, 113, 174	0
11	I	127/128 (99%)	0.91	16 (12%) 8 7	35, 90, 149, 178	0
12	J	98/105 (93%)	1.67	35 (35%) 1 1	44, 117, 186, 200	0
13	K	119/129 (92%)	0.36	8 (6%) 24 16	30, 67, 138, 187	0
14	L	124/135 (91%)	0.57	13 (10%) 11 9	31, 64, 139, 175	0
15	M	125/126 (99%)	1.00	17 (13%) 7 6	44, 85, 169, 200	0
16	N	60/61 (98%)	0.88	5 (8%) 17 13	42, 82, 139, 179	0
17	O	88/89 (98%)	0.55	8 (9%) 15 11	23, 76, 142, 192	0
18	P	83/88 (94%)	0.26	3 (3%) 46 31	27, 52, 96, 173	0
19	Q	104/105 (99%)	0.55	9 (8%) 16 12	22, 61, 146, 200	0
20	R	73/88 (82%)	0.49	4 (5%) 30 21	40, 79, 175, 188	0
21	S	80/93 (86%)	1.19	15 (18%) 3 3	62, 111, 162, 193	0
22	T	99/106 (93%)	0.54	9 (9%) 15 11	32, 58, 136, 168	0
23	V	24/27 (88%)	1.23	6 (25%) 2 1	41, 69, 118, 136	0
All	All	3915/4077 (96%)	0.74	473 (12%) 8 7	20, 73, 159, 200	0

The worst 5 of 473 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	217	C	8.6
19	Q	102	GLY	8.3
1	A	409	G	8.3
1	A	216	G	8.1
1	A	202	U	8.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
3	T6A	X	37	32/33	0.88	0.18	76,80,80,80	0
3	MNU	X	34	23/24	0.89	0.18	56,96,115,115	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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
25	MG	A	1619	1/1	0.45	0.40	23,23,23,23	1
25	MG	A	1631	1/1	0.66	0.21	23,23,23,23	1
25	MG	A	1550	1/1	0.72	0.27	23,23,23,23	1
25	MG	A	1615	1/1	0.74	0.41	23,23,23,23	1
25	MG	A	214	1/1	0.75	0.44	23,23,23,23	1
25	MG	A	210	1/1	0.75	0.21	23,23,23,23	1
25	MG	A	1562	1/1	0.79	0.48	23,23,23,23	1
25	MG	A	1621	1/1	0.81	0.20	23,23,23,23	1
25	MG	A	1548	1/1	0.82	0.37	23,23,23,23	1
25	MG	A	1575	1/1	0.82	0.53	23,23,23,23	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	MG	A	1628	1/1	0.83	0.25	23,23,23,23	1
25	MG	A	1591	1/1	0.83	0.39	23,23,23,23	1
25	MG	A	1607	1/1	0.84	0.56	23,23,23,23	1
25	MG	A	1582	1/1	0.86	0.19	23,23,23,23	0
25	MG	A	1570	1/1	0.87	0.24	23,23,23,23	0
25	MG	A	1623	1/1	0.87	0.40	23,23,23,23	1
25	MG	A	1588	1/1	0.88	0.35	23,23,23,23	0
25	MG	A	1584	1/1	0.88	0.24	23,23,23,23	0
25	MG	A	1625	1/1	0.88	0.30	23,23,23,23	1
25	MG	A	1616	1/1	0.88	0.15	23,23,23,23	1
25	MG	A	1599	1/1	0.88	0.22	23,23,23,23	1
25	MG	A	1635	1/1	0.88	0.41	23,23,23,23	1
25	MG	A	1614	1/1	0.89	0.26	23,23,23,23	1
25	MG	A	441	1/1	0.89	0.20	23,23,23,23	1
25	MG	A	471	1/1	0.89	0.26	23,23,23,23	1
25	MG	A	1605	1/1	0.89	0.26	23,23,23,23	1
25	MG	A	493	1/1	0.89	0.55	23,23,23,23	1
25	MG	A	86	1/1	0.89	0.14	23,23,23,23	1
25	MG	A	1571	1/1	0.90	0.16	23,23,23,23	0
25	MG	A	1630	1/1	0.90	0.17	23,23,23,23	1
25	MG	A	469	1/1	0.90	0.20	23,23,23,23	1
25	MG	A	1564	1/1	0.90	0.18	23,23,23,23	0
25	MG	A	473	1/1	0.90	0.58	23,23,23,23	1
25	MG	A	1561	1/1	0.90	0.13	23,23,23,23	1
25	MG	A	1551	1/1	0.90	0.30	23,23,23,23	0
25	MG	A	1586	1/1	0.90	0.21	23,23,23,23	1
25	MG	A	1566	1/1	0.91	0.37	23,23,23,23	1
25	MG	A	1622	1/1	0.91	0.56	23,23,23,23	1
24	PAR	A	1545	42/42	0.91	0.12	25,25,25,25	0
25	MG	A	1600	1/1	0.91	0.23	23,23,23,23	1
25	MG	A	1568	1/1	0.91	0.13	23,23,23,23	0
25	MG	A	1565	1/1	0.91	0.13	23,23,23,23	0
25	MG	A	1603	1/1	0.92	0.28	23,23,23,23	1
25	MG	A	1574	1/1	0.92	0.19	23,23,23,23	0
25	MG	A	1595	1/1	0.92	0.39	23,23,23,23	1
25	MG	A	1560	1/1	0.92	0.25	23,23,23,23	0
25	MG	A	1579	1/1	0.92	0.18	23,23,23,23	1
25	MG	A	466	1/1	0.93	0.28	23,23,23,23	1
25	MG	A	467	1/1	0.93	0.13	23,23,23,23	1
25	MG	A	1610	1/1	0.93	0.34	23,23,23,23	1
25	MG	A	1576	1/1	0.93	0.18	23,23,23,23	0
25	MG	A	1577	1/1	0.93	0.10	23,23,23,23	0

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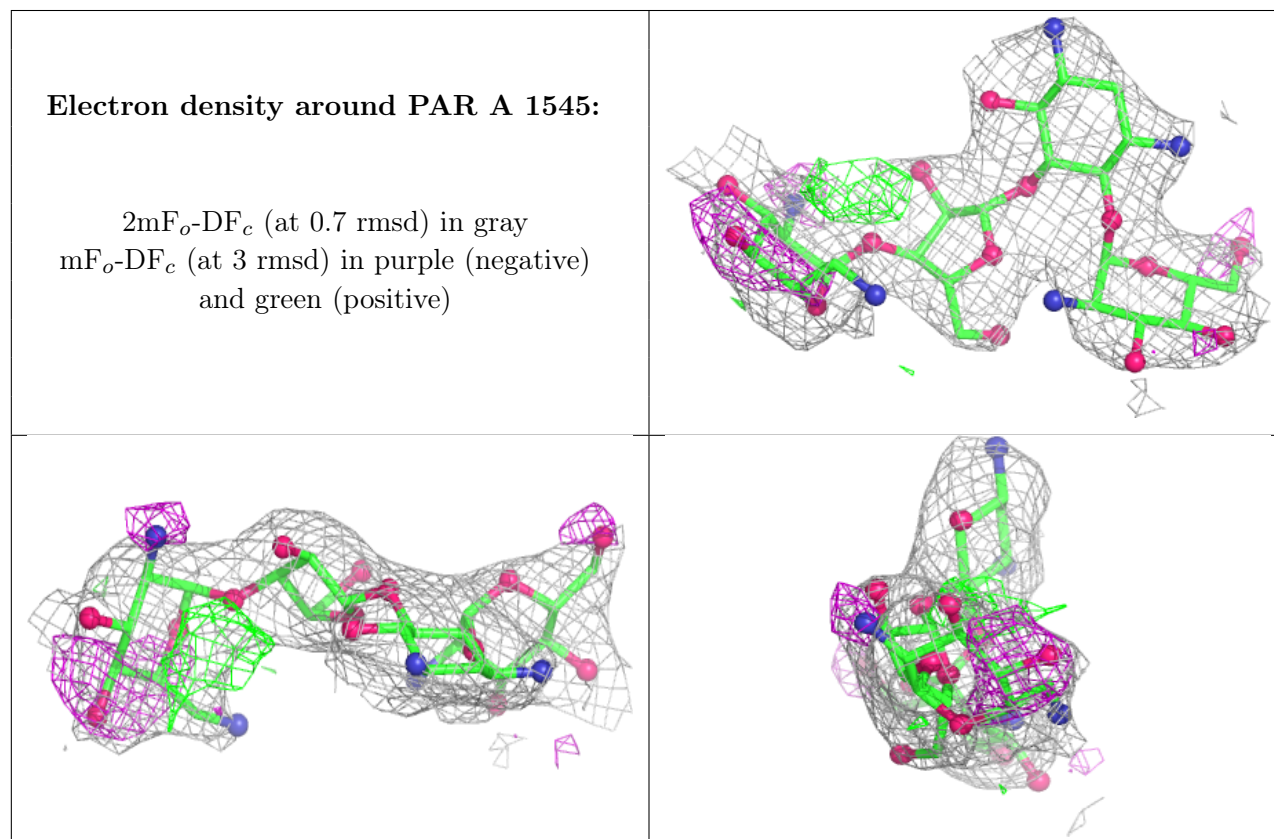
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	MG	A	1547	1/1	0.93	0.18	23,23,23,23	0
25	MG	A	1632	1/1	0.93	0.15	23,23,23,23	1
25	MG	A	1606	1/1	0.93	0.07	23,23,23,23	1
25	MG	A	1559	1/1	0.93	0.22	23,23,23,23	0
25	MG	A	211	1/1	0.94	0.32	23,23,23,23	0
25	MG	A	1620	1/1	0.94	0.21	23,23,23,23	1
25	MG	A	1546	1/1	0.94	0.21	23,23,23,23	0
25	MG	A	1590	1/1	0.94	0.20	23,23,23,23	0
25	MG	A	1596	1/1	0.94	0.56	23,23,23,23	1
25	MG	A	1569	1/1	0.94	0.24	23,23,23,23	1
25	MG	A	1624	1/1	0.94	0.23	23,23,23,23	1
25	MG	A	1592	1/1	0.94	0.09	23,23,23,23	0
25	MG	A	1626	1/1	0.94	0.17	23,23,23,23	1
25	MG	A	1554	1/1	0.94	0.49	23,23,23,23	1
25	MG	X	502	1/1	0.94	0.46	23,23,23,23	1
25	MG	A	1617	1/1	0.95	0.21	23,23,23,23	1
25	MG	A	1618	1/1	0.95	0.10	23,23,23,23	0
25	MG	A	1558	1/1	0.95	0.07	23,23,23,23	0
25	MG	A	1602	1/1	0.95	0.20	23,23,23,23	0
25	MG	A	1627	1/1	0.95	0.19	23,23,23,23	1
25	MG	A	1587	1/1	0.95	0.19	23,23,23,23	0
25	MG	A	1634	1/1	0.95	0.38	23,23,23,23	1
25	MG	A	1629	1/1	0.95	0.18	23,23,23,23	0
25	MG	A	87	1/1	0.95	0.33	23,23,23,23	1
25	MG	A	1578	1/1	0.95	0.10	23,23,23,23	0
25	MG	J	449	1/1	0.95	0.11	23,23,23,23	1
25	MG	A	1563	1/1	0.96	0.22	23,23,23,23	1
25	MG	A	71	1/1	0.96	0.24	23,23,23,23	1
25	MG	A	1581	1/1	0.96	0.40	23,23,23,23	1
25	MG	A	1608	1/1	0.96	0.29	23,23,23,23	1
25	MG	A	1557	1/1	0.96	0.13	23,23,23,23	0
25	MG	A	1611	1/1	0.96	0.09	23,23,23,23	1
25	MG	A	1552	1/1	0.97	0.16	23,23,23,23	0
25	MG	A	1572	1/1	0.97	0.11	23,23,23,23	0
25	MG	A	1573	1/1	0.97	0.14	23,23,23,23	0
25	MG	A	470	1/1	0.97	0.21	23,23,23,23	1
25	MG	A	1597	1/1	0.97	0.06	23,23,23,23	1
25	MG	A	1598	1/1	0.97	0.06	23,23,23,23	0
25	MG	A	1613	1/1	0.97	0.17	23,23,23,23	1
25	MG	A	1580	1/1	0.97	0.24	23,23,23,23	1
25	MG	A	1549	1/1	0.97	0.25	23,23,23,23	1
25	MG	A	1555	1/1	0.97	0.26	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	MG	A	1556	1/1	0.97	0.17	23,23,23,23	0
25	MG	X	500	1/1	0.97	0.11	23,23,23,23	1
25	MG	A	1604	1/1	0.97	0.21	23,23,23,23	1
25	MG	A	1585	1/1	0.97	0.32	23,23,23,23	1
25	MG	A	1567	1/1	0.98	0.28	23,23,23,23	0
25	MG	A	1633	1/1	0.98	0.40	23,23,23,23	1
25	MG	A	1612	1/1	0.98	0.14	23,23,23,23	1
25	MG	A	1601	1/1	0.98	0.07	23,23,23,23	1
25	MG	A	1589	1/1	0.98	0.24	23,23,23,23	0
25	MG	A	1593	1/1	0.98	0.30	23,23,23,23	1
25	MG	A	1609	1/1	0.98	0.17	23,23,23,23	0
25	MG	A	1583	1/1	0.98	0.12	23,23,23,23	0
26	ZN	D	306	1/1	0.98	0.12	23,23,23,23	1
25	MG	A	1594	1/1	0.99	0.06	23,23,23,23	1
25	MG	A	1553	1/1	0.99	0.19	23,23,23,23	0
26	ZN	N	307	1/1	1.00	0.04	23,23,23,23	1

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.