



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 07:16 AM UTC

PDB ID : 4OX9 / pdb_00004ox9
Title : Crystal structure of the aminoglycoside resistance methyltransferase NpmA bound to the 30S ribosomal subunit
Authors : Dunkle, J.A.; Conn, G.L.; Dunham, C.M.
Deposited on : 2014-02-04
Resolution : 3.80 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

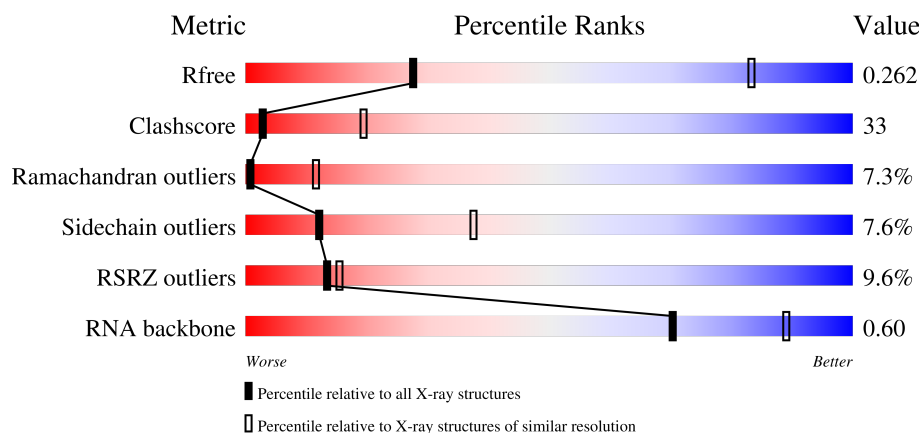
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)
RNA backbone	3983	1007 (4.50-3.10)

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	1513	6% 32% 52% 12% .
2	B	256	10% 24% 50% 15% . 9%
3	C	239	11% 25% 43% 16% . 14%
4	D	208	10% 38% 51% 10%

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Mol	Chain	Length	Quality of chain
5	E	161	
6	F	101	
7	G	155	
8	H	138	
9	I	128	
10	J	104	
11	K	129	
12	L	131	
13	M	126	
14	N	60	
15	O	88	
16	P	88	
17	Q	104	
18	R	88	
19	S	92	
20	T	106	
21	V	26	
22	Y	222	

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
23	MG	A	1604	-	-	-	X
23	MG	A	1611	-	-	-	X
23	MG	A	1620	-	-	-	X
23	MG	A	1621	-	-	-	X
23	MG	A	1624	-	-	-	X
23	MG	A	1626	-	-	-	X
23	MG	A	1629	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	MG	A	1637	-	-	-	X
23	MG	A	1647	-	-	-	X
23	MG	A	1650	-	-	-	X
23	MG	A	1652	-	-	-	X
23	MG	A	1677	-	-	-	X
23	MG	A	1699	-	-	-	X
23	MG	A	1703	-	-	-	X
23	MG	N	102	-	-	-	X

2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 53527 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 rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1507	Total	C	N	O	P	0	0	0
			32394	14418	6002	10467	1507			

- Molecule 2 is a protein called 30S ribosomal protein S2.

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

- Molecule 3 is a protein called 30S ribosomal protein S3.

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

- Molecule 4 is a protein called 30S ribosomal protein S4.

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

- Molecule 5 is a protein called 30S ribosomal protein S5.

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

- Molecule 6 is a protein called 30S ribosomal protein S6.

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

- Molecule 7 is a protein called 30S ribosomal protein S7.

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

- Molecule 8 is a protein called 30S ribosomal protein S8.

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

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	127	Total	C	N	O	S	0	0	0
			1010	639	197	174				

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	98	Total	C	N	O	S	0	0	0
			785	494	153	137	1			

- Molecule 11 is a protein called 30S ribosomal protein S11.

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

- Molecule 12 is a protein called 30S ribosomal protein S12.

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

- Molecule 13 is a protein called 30S ribosomal protein S13.

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

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

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

- Molecule 15 is a protein called 30S ribosomal protein S15.

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

- Molecule 16 is a protein called 30S ribosomal protein S16.

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

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	104	Total	C	N	O	S	0	0	0
			857	547	160	148	2			

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	73	Total	C	N	O	0	0	0
			598	381	118	99			

- Molecule 19 is a protein called 30S ribosomal protein S19.

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

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

- Molecule 21 is a protein called 30S ribosomal protein Thx.

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

- Molecule 22 is a protein called 16S rRNA (adenine(1408)-N(1))-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	Y	219	Total	C	N	O	S	0	0	0
			1761	1138	294	328	1			

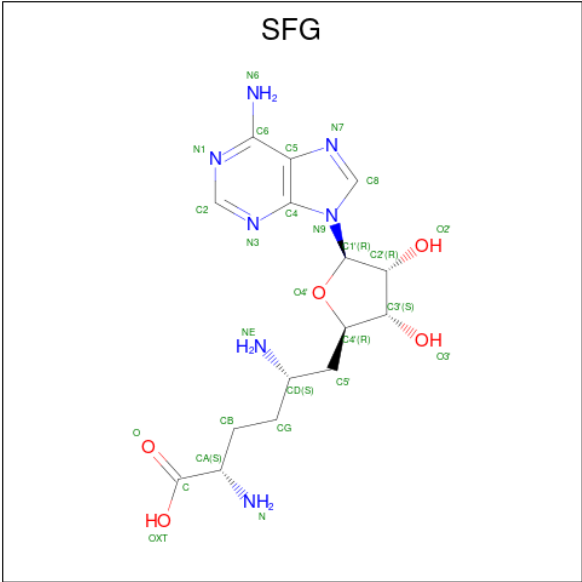
- Molecule 23 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	A	117	Total	Mg	0	0
			117	117		
23	B	1	Total	Mg	0	0
			1	1		
23	E	1	Total	Mg	0	0
			1	1		
23	N	1	Total	Mg	0	0
			1	1		

- Molecule 24 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 25 is SINEFUNGIN (CCD ID: SFG) (formula: C₁₅H₂₃N₇O₅).

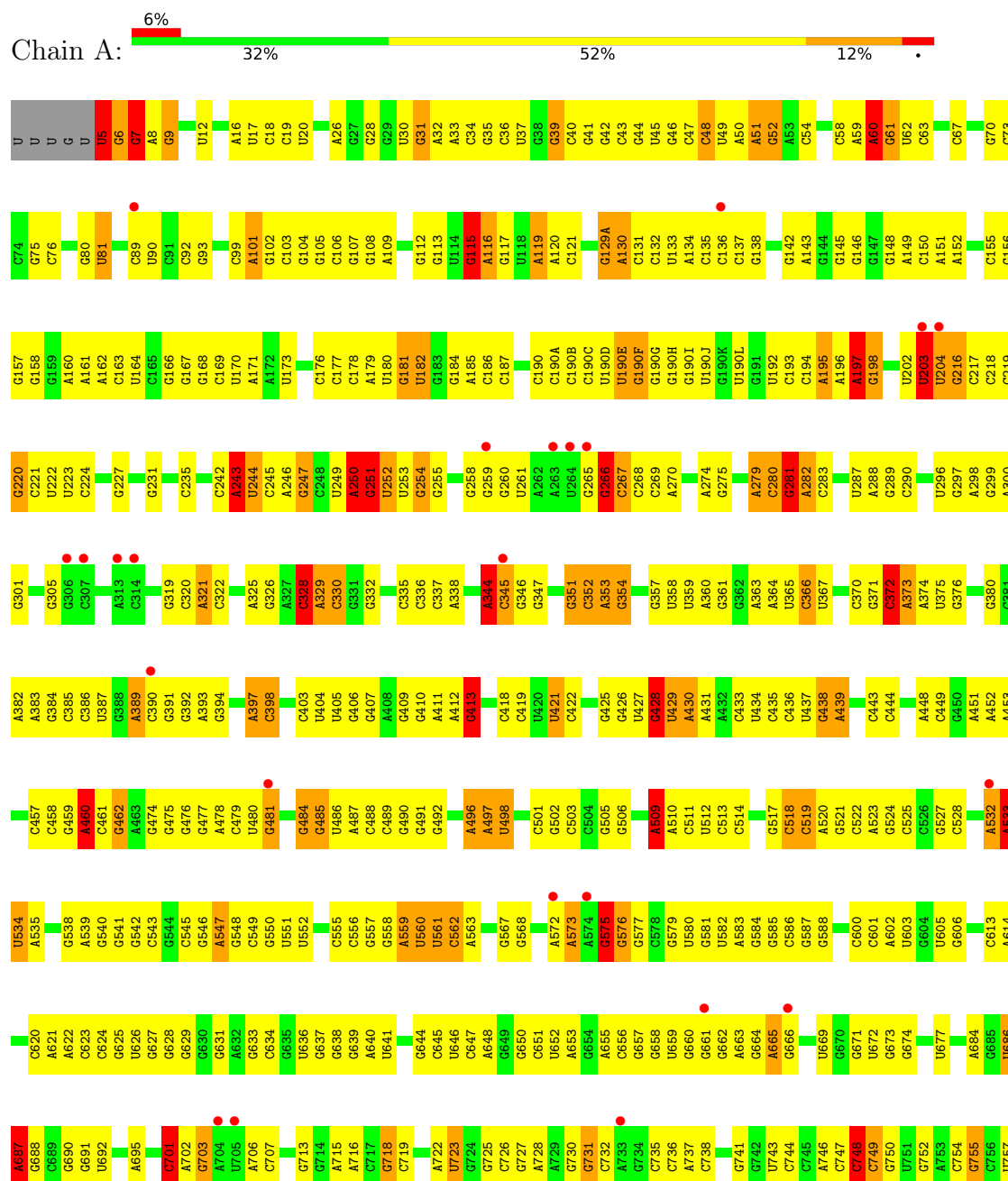


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	Y	1	Total	C	N	O	0	0
			27	15	7	5		

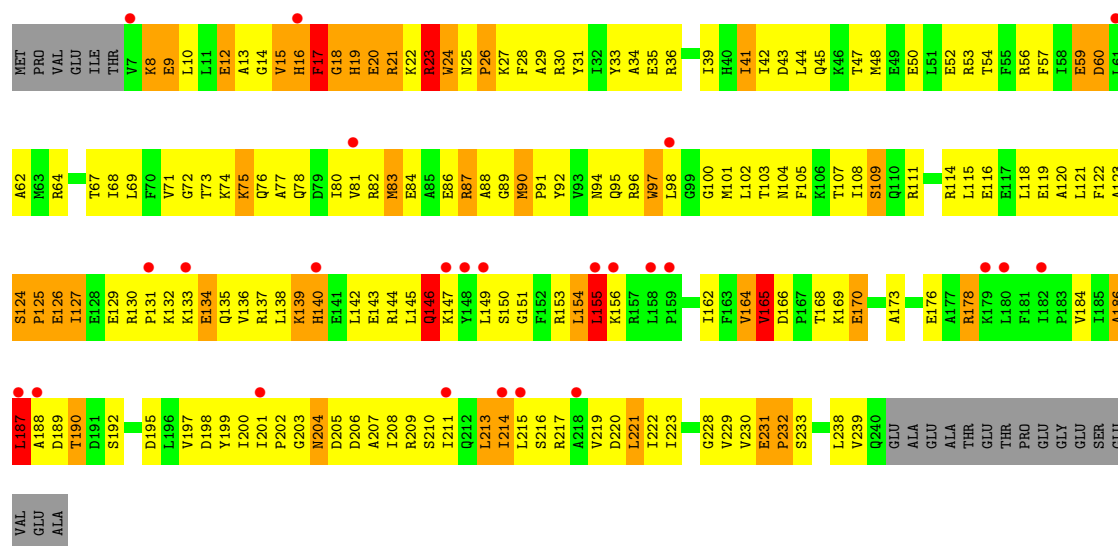
3 Residue-property plots

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

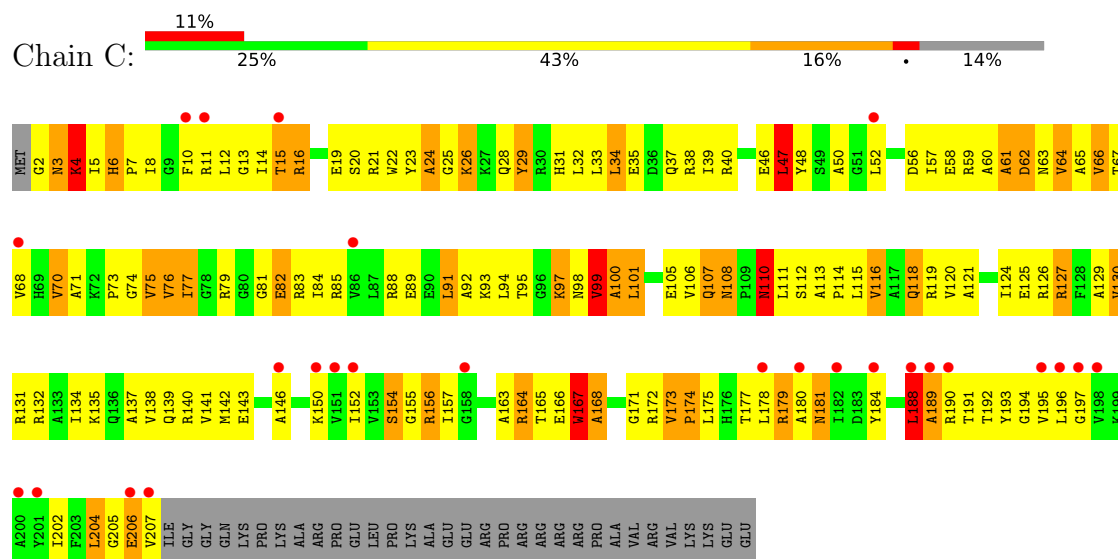
• Molecule 1: 16S rRNA



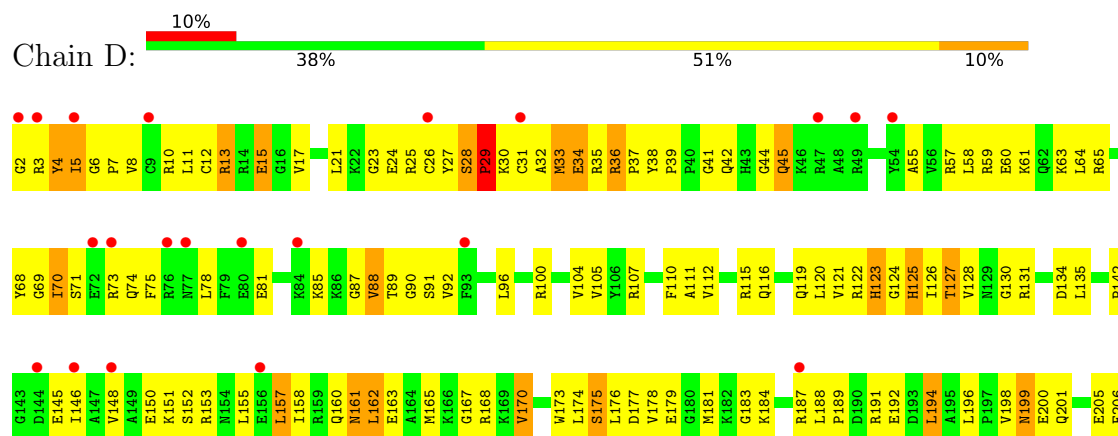




• Molecule 3: 30S ribosomal protein S3



• Molecule 4: 30S ribosomal protein S4



Y207
S208
R209

• Molecule 5: 30S ribosomal protein S5

Chain E: 

PRO GLU THR D5 F6 E7 M10 I11 I12 I13 I14 I15 I16 I17 I18 I19 M20 Q20 Q21 A21 G22 G23 G24 R25 R26 R27 A30 A31 D36 D37 Q38 G39 R40 V41 G42 G43 G44 F45 G46 R47 V51 P52 L53 A54 V55 Q56 K57 A58 G59 Y61 R64 R65 R66 R67 R68 V69

P70 L71 G74 I76 P77 E78 E79 I80 E81 E82 E83 I89 V90 L91 L92 K92 P93 I101 G102 G103 A104 V105 P106 R107 A108 V115 T116 D117 I118 L119 T120 K121 E122 L123 G124 S125 R126 N127 P128 I131 A132 M136 E137 Q141 L142 R143 T144 K145 A146 D147 V148 E149 R150

L151 R152 K153 G154 ALA ALA HIS ALA ALA ALA GLY

• Molecule 6: 30S ribosomal protein S6

Chain F: 

H1 R2 R3 Y4 V6 V7 W8 W9 L10 L15 Q16 L19 A20 L21 E22 E23 E24 E25 L26 L30 Y33 G34 A35 R36 V37 E38 K39 V40 E41 E42 L43 G44 L45 R46 R47 L48 A49 Y50 P51 L52 A53 K54 D55 P56 Q57 G58 Y59 F60 Y63 G64 R65 E66 M67 P68

E69 D70 R71 W72 D74 L75 A76 R77 L78 L79 R80 R81 R82 R83 R84 R85 R86 R87 R88 R89 V90 V91 K92 S93 Q94 E95 P96 F97 M100 A101

• Molecule 7: 30S ribosomal protein S7

Chain G: 

A2 R3 R4 R5 R6 A7 E8 V9 R10 Q11 Q12 Q13 Q14 D15 L16 V17 Y18 G19 D20 V21 L22 V23 V24 A25 F26 I27 I30 M31 G34 L38 A39 E40 I41 I42 F43 Y44 D45 A46 I49 I50 Q51 E52 K53 T54 G55 Q56 L59 Q64 A65 V66 E67 R68 K70

P71 R72 V75 S77 R78 R79 R80 G81 G82 A83 R84 R85 Q86 R87 P93 R94 R95 A100 L101 R102 W103 L104 V105 Q106 A107 A108 H109 G110 R111 P112 E113 R114 R115 A116 A117 V118 R119 I120 A121 H122 M125 A134 V135 K138 E139 E142 R143 W144 A145 E146 R147 V148 N148

R149 A150 Y154 R155 A156

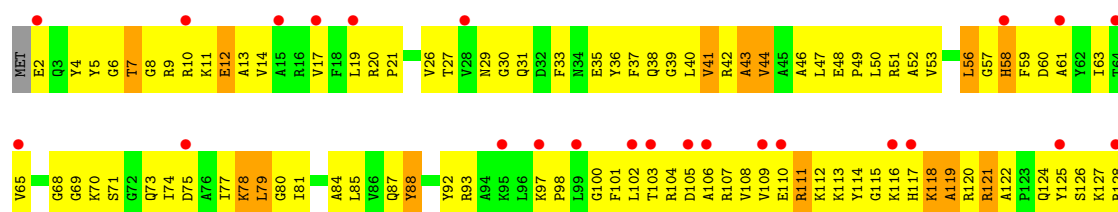
• Molecule 8: 30S ribosomal protein S8

Chain H: 

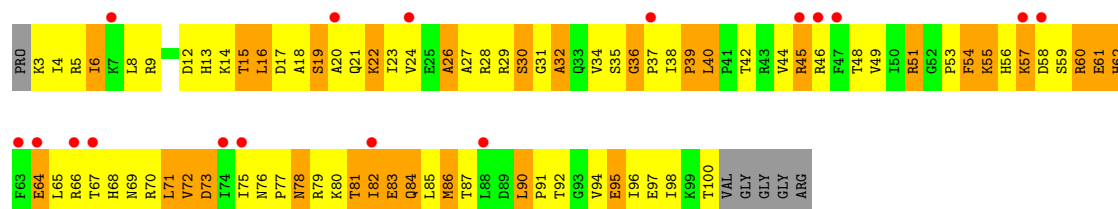
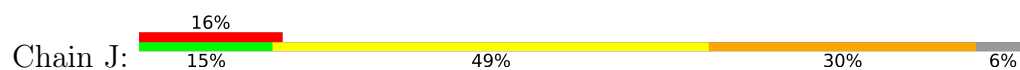
M1 L2 T3 I6 A7 D8 M9 L10 T11 T12 I13 I14 I15 A16 A17 R18 R19 V19 Y20 K21 E22 S23 S24 V25 V26 S29 R30 F31 K32 I35 L36 R37 I38 L39 I45 E49 R50 V51 D52 K56 L59 R60 V61 Y62 L63 K64 Y65 R68 D73 P74 R75 R76 P77



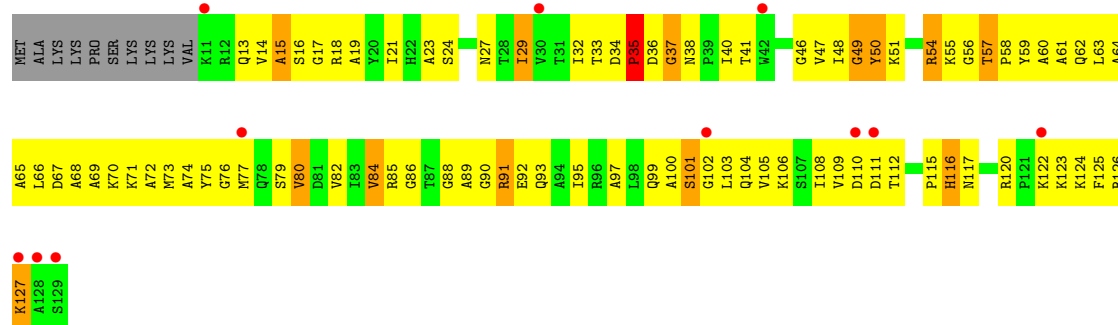
• Molecule 9: 30S ribosomal protein S9



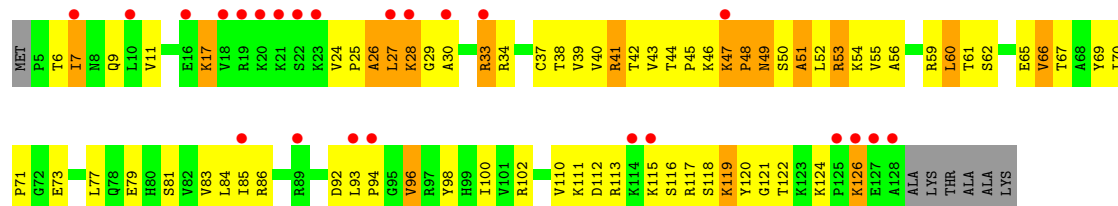
• Molecule 10: 30S ribosomal protein S10



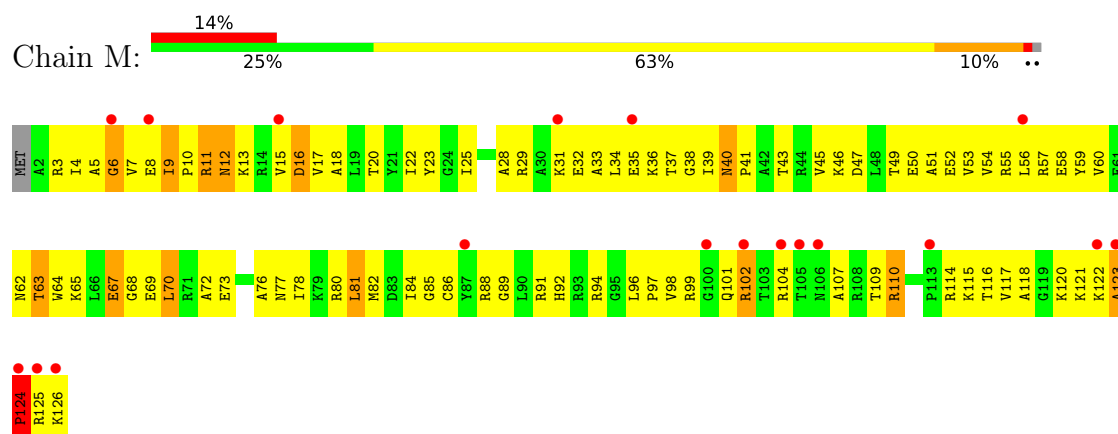
• Molecule 11: 30S ribosomal protein S11



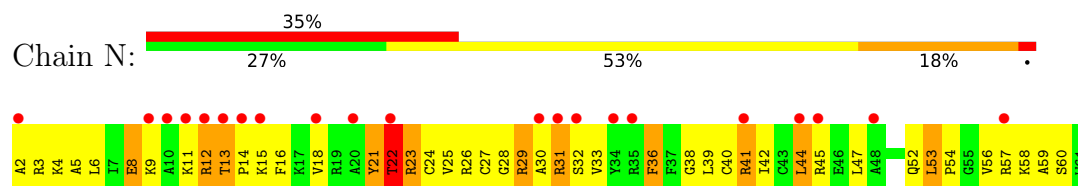
• Molecule 12: 30S ribosomal protein S12



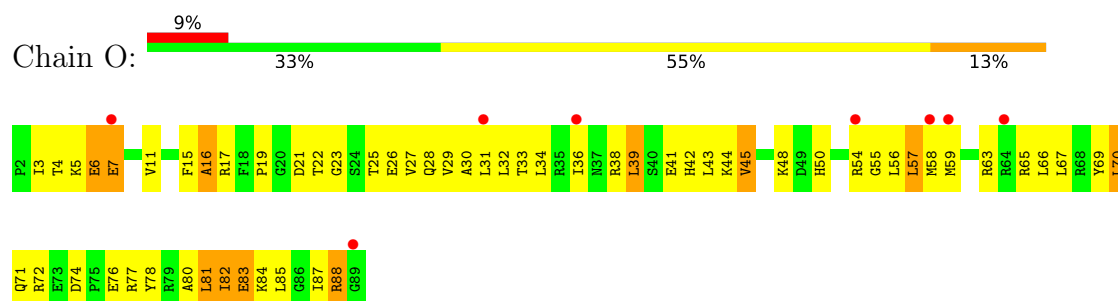
- Molecule 13: 30S ribosomal protein S13



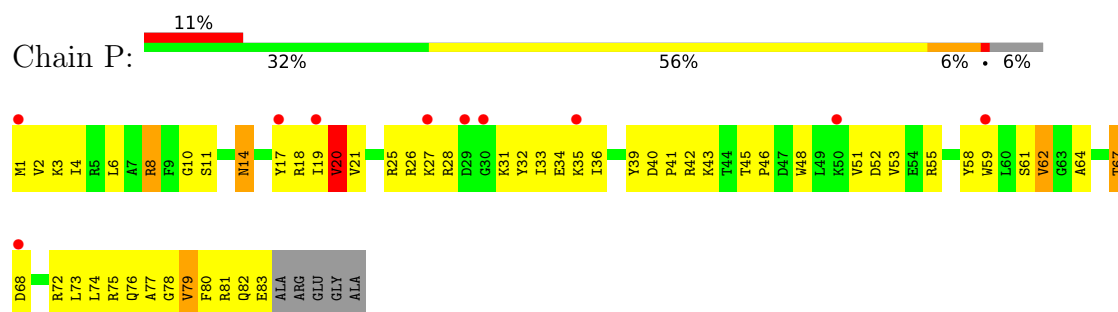
- Molecule 14: 30S ribosomal protein S14 type Z



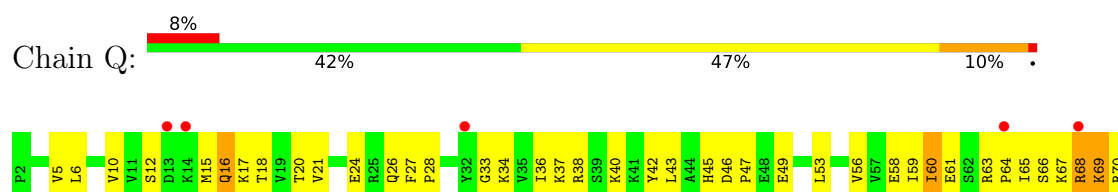
- Molecule 15: 30S ribosomal protein S15



- Molecule 16: 30S ribosomal protein S16

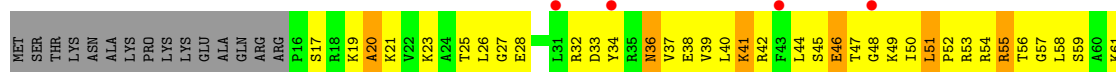
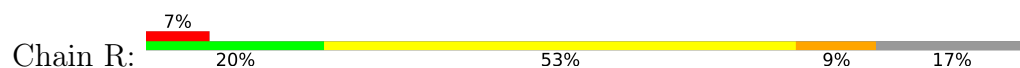


- Molecule 17: 30S ribosomal protein S17

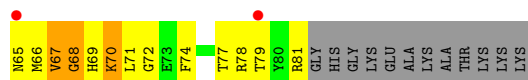
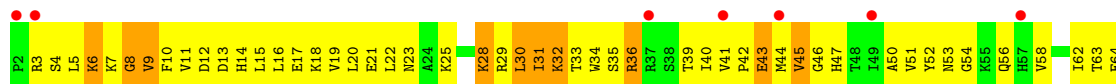
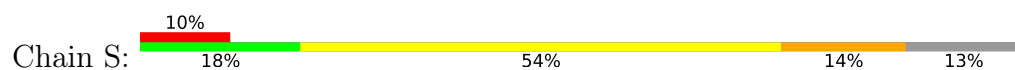


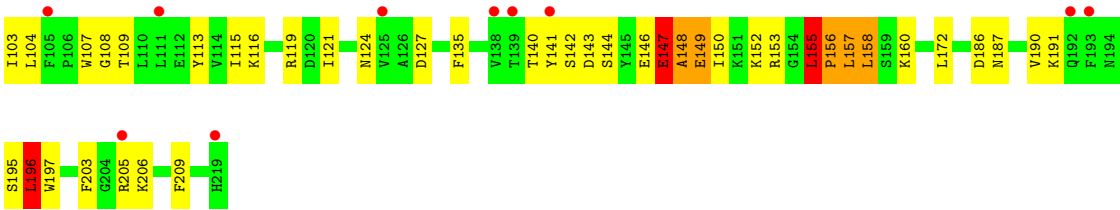


• Molecule 18: 30S ribosomal protein S18



• Molecule 19: 30S ribosomal protein S19





4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	403.52Å 403.52Å 176.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.72 – 3.80 49.72 – 3.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.72-3.80) 94.0 (49.72-3.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 3.77Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.233 , 0.257 0.238 , 0.262	Depositor DCC
R_{free} test set	7034 reflections (2.60%)	wwPDB-VP
Wilson B-factor (Å ²)	132.9	Xtriage
Anisotropy	0.320	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 60.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	53527	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.52% 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: SFG, ZN, 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	0.43	0/36262	0.72	79/56597 (0.1%)
2	B	0.56	4/1935 (0.2%)	1.10	17/2609 (0.7%)
3	C	0.54	3/1636 (0.2%)	1.04	11/2205 (0.5%)
4	D	0.53	4/1733 (0.2%)	0.96	7/2318 (0.3%)
5	E	0.92	2/1162 (0.2%)	1.23	14/1564 (0.9%)
6	F	0.53	1/856 (0.1%)	0.96	3/1154 (0.3%)
7	G	0.46	1/1276 (0.1%)	1.00	6/1709 (0.4%)
8	H	0.58	0/1136	1.13	9/1527 (0.6%)
9	I	0.41	0/1029	0.94	4/1379 (0.3%)
10	J	0.62	3/798 (0.4%)	1.13	8/1073 (0.7%)
11	K	0.51	0/900	1.07	4/1213 (0.3%)
12	L	0.52	0/986	1.08	4/1320 (0.3%)
13	M	0.50	1/1008 (0.1%)	0.99	2/1347 (0.1%)
14	N	0.44	0/501	1.21	7/664 (1.1%)
15	O	0.48	0/745	0.95	3/992 (0.3%)
16	P	0.52	0/716	1.17	8/963 (0.8%)
17	Q	0.59	1/870 (0.1%)	1.07	2/1159 (0.2%)
18	R	0.52	1/604 (0.2%)	0.97	4/801 (0.5%)
19	S	0.42	0/661	1.10	5/890 (0.6%)
20	T	0.58	1/765 (0.1%)	1.14	7/1007 (0.7%)
21	V	0.49	0/212	0.87	0/277
22	Y	0.62	0/1796	1.29	11/2418 (0.5%)
All	All	0.48	22/57587 (0.0%)	0.86	215/85186 (0.3%)

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	0	41

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Mol	Chain	#Chirality outliers	#Planarity outliers
22	Y	0	2
All	All	0	43

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	101	ILE	C-N	19.49	1.58	1.33
5	E	69	VAL	C-N	9.33	1.55	1.33
2	B	19	HIS	ND1-CE1	5.30	1.37	1.32
13	M	40	ASN	CG-OD1	5.26	1.33	1.23
17	Q	16	GLN	CD-OE1	5.26	1.33	1.23

The worst 5 of 215 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	Y	155	LEU	CA-C-N	16.01	136.27	119.78
22	Y	155	LEU	C-N-CA	16.01	136.27	119.78
1	A	1498	U	C2'-C3'-O3'	14.53	131.29	109.50
1	A	243	A	C2'-C3'-O3'	13.88	130.32	109.50
1	A	559	A	C2'-C3'-O3'	13.42	129.63	109.50

There are no chirality outliers.

5 of 43 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	12	U	Sidechain
1	A	197	A	Sidechain
1	A	203	U	Sidechain
1	A	220	G	Sidechain
1	A	231	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	32394	0	16349	1175	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1900	0	1951	223	0
3	C	1612	0	1677	224	0
4	D	1703	0	1764	143	0
5	E	1146	0	1207	108	0
6	F	843	0	857	70	0
7	G	1257	0	1296	95	0
8	H	1116	0	1177	70	0
9	I	1010	0	1037	119	0
10	J	785	0	823	128	0
11	K	885	0	904	88	0
12	L	970	0	1057	110	0
13	M	997	0	1072	122	0
14	N	492	0	529	76	0
15	O	734	0	771	64	0
16	P	700	0	720	59	0
17	Q	857	0	928	89	0
18	R	598	0	670	62	0
19	S	647	0	673	86	0
20	T	763	0	860	92	0
21	V	208	0	221	29	0
22	Y	1761	0	1792	51	0
23	A	117	0	0	0	0
23	B	1	0	0	0	0
23	E	1	0	0	0	0
23	N	1	0	0	0	0
24	D	1	0	0	0	0
24	N	1	0	0	0	0
25	Y	27	0	22	4	0
All	All	53527	0	38357	2996	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 33.

The worst 5 of 2996 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:57:GLY:O	9:I:58:HIS:HD2	1.22	1.18
20:T:54:LYS:HG3	20:T:100:ILE:CD1	1.73	1.18
12:L:41:ARG:HG2	12:L:42:THR:H	1.03	1.15
9:I:57:GLY:O	9:I:58:HIS:CD2	2.00	1.14
2:B:77:ALA:HB2	2:B:211:ILE:HD13	1.22	1.14

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	232/256 (91%)	174 (75%)	34 (15%)	24 (10%)	0	6
3	C	204/239 (85%)	135 (66%)	41 (20%)	28 (14%)	0	3
4	D	206/208 (99%)	166 (81%)	31 (15%)	9 (4%)	2	19
5	E	148/161 (92%)	130 (88%)	13 (9%)	5 (3%)	3	23
6	F	99/101 (98%)	79 (80%)	19 (19%)	1 (1%)	12	43
7	G	153/155 (99%)	127 (83%)	16 (10%)	10 (6%)	1	14
8	H	136/138 (99%)	125 (92%)	7 (5%)	4 (3%)	3	25
9	I	125/128 (98%)	88 (70%)	27 (22%)	10 (8%)	1	10
10	J	96/104 (92%)	59 (62%)	20 (21%)	17 (18%)	0	2
11	K	117/129 (91%)	88 (75%)	20 (17%)	9 (8%)	1	11
12	L	122/131 (93%)	97 (80%)	16 (13%)	9 (7%)	1	11
13	M	123/126 (98%)	88 (72%)	27 (22%)	8 (6%)	1	14
14	N	58/60 (97%)	40 (69%)	11 (19%)	7 (12%)	0	4
15	O	86/88 (98%)	70 (81%)	11 (13%)	5 (6%)	1	15
16	P	81/88 (92%)	65 (80%)	15 (18%)	1 (1%)	10	40
17	Q	102/104 (98%)	84 (82%)	10 (10%)	8 (8%)	1	11
18	R	71/88 (81%)	62 (87%)	7 (10%)	2 (3%)	4	26
19	S	78/92 (85%)	49 (63%)	18 (23%)	11 (14%)	0	3
20	T	97/106 (92%)	63 (65%)	21 (22%)	13 (13%)	0	3
21	V	22/26 (85%)	19 (86%)	2 (9%)	1 (4%)	2	18
22	Y	217/222 (98%)	206 (95%)	6 (3%)	5 (2%)	5	30
All	All	2573/2750 (94%)	2014 (78%)	372 (14%)	187 (7%)	1	11

5 of 187 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	9	GLU
2	B	15	VAL
2	B	16	HIS
2	B	17	PHE
2	B	21	ARG

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	
2	B	202/220 (92%)	184 (91%)	18 (9%)	9	32
3	C	160/188 (85%)	141 (88%)	19 (12%)	5	22
4	D	180/180 (100%)	169 (94%)	11 (6%)	17	43
5	E	115/122 (94%)	98 (85%)	17 (15%)	3	16
6	F	90/90 (100%)	85 (94%)	5 (6%)	19	45
7	G	126/126 (100%)	121 (96%)	5 (4%)	28	52
8	H	119/119 (100%)	107 (90%)	12 (10%)	7	27
9	I	98/99 (99%)	91 (93%)	7 (7%)	13	39
10	J	86/91 (94%)	77 (90%)	9 (10%)	6	26
11	K	90/99 (91%)	83 (92%)	7 (8%)	11	36
12	L	104/108 (96%)	95 (91%)	9 (9%)	9	33
13	M	100/101 (99%)	92 (92%)	8 (8%)	11	36
14	N	49/49 (100%)	47 (96%)	2 (4%)	27	51
15	O	79/79 (100%)	72 (91%)	7 (9%)	9	32
16	P	72/74 (97%)	67 (93%)	5 (7%)	14	40
17	Q	96/96 (100%)	90 (94%)	6 (6%)	16	42
18	R	64/77 (83%)	60 (94%)	4 (6%)	16	42
19	S	71/79 (90%)	70 (99%)	1 (1%)	59	70
20	T	76/82 (93%)	69 (91%)	7 (9%)	8	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	V	19/21 (90%)	19 (100%)	0	100	100
22	Y	193/195 (99%)	186 (96%)	7 (4%)	31	54
All	All	2189/2295 (95%)	2023 (92%)	166 (8%)	12	37

5 of 166 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	L	81	SER
17	Q	60	ILE
13	M	9	ILE
15	O	7	GLU
18	R	75	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
10	J	69	ASN
12	L	8	ASN
22	Y	134	HIS
13	M	77	ASN
3	C	107	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1507/1513 (99%)	230 (15%)	90 (5%)

5 of 230 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	8	A
1	A	9	G
1	A	31	G
1	A	32	A

5 of 90 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1101	A
1	A	1281	U
1	A	1145	C
1	A	1214	C
1	A	1302	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 123 ligands modelled in this entry, 122 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
25	SFG	Y	301	-	28,29,29	0.82	0	34,42,42	1.99	7 (20%)

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
25	SFG	Y	301	-	-	4/17/33/33	0/3/3/3

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Y	301	SFG	C5-C4-N3	-5.60	119.01	126.72
25	Y	301	SFG	N3-C4-N9	4.53	134.87	127.17
25	Y	301	SFG	N3-C2-N1	-4.06	122.44	128.58
25	Y	301	SFG	C5-N7-C8	3.81	109.43	103.45
25	Y	301	SFG	C2-N3-C4	3.63	120.70	111.83

There are no chirality outliers.

All (4) torsion outliers are listed below:

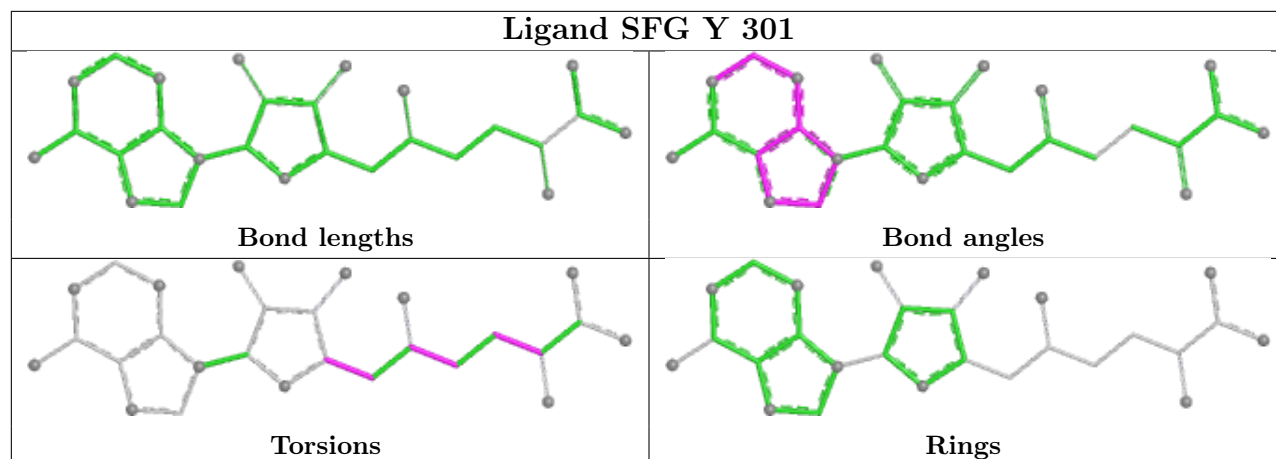
Mol	Chain	Res	Type	Atoms
25	Y	301	SFG	C5'-CD-CG-CB
25	Y	301	SFG	N-CA-CB-CG
25	Y	301	SFG	C-CA-CB-CG
25	Y	301	SFG	C3'-C4'-C5'-CD

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	Y	301	SFG	4	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	1507/1513 (99%)	0.43	95 (6%) 26 21	18, 71, 170, 260	0
2	B	234/256 (91%)	0.72	25 (10%) 11 14	29, 94, 152, 190	0
3	C	206/239 (86%)	0.72	26 (12%) 8 11	44, 104, 145, 171	0
4	D	208/208 (100%)	0.74	21 (10%) 12 14	25, 79, 127, 182	0
5	E	150/161 (93%)	0.23	5 (3%) 49 34	18, 56, 106, 148	0
6	F	101/101 (100%)	0.53	8 (7%) 18 17	48, 103, 142, 156	0
7	G	155/155 (100%)	0.37	9 (5%) 29 23	40, 96, 148, 172	0
8	H	138/138 (100%)	0.40	5 (3%) 46 32	11, 41, 81, 116	0
9	I	127/128 (99%)	1.04	24 (18%) 3 5	40, 105, 144, 165	0
10	J	98/104 (94%)	1.15	17 (17%) 4 6	55, 123, 165, 188	0
11	K	119/129 (92%)	0.79	11 (9%) 14 16	36, 81, 129, 171	0
12	L	124/131 (94%)	1.09	24 (19%) 3 5	18, 74, 120, 165	0
13	M	125/126 (99%)	0.95	18 (14%) 6 9	56, 97, 137, 185	0
14	N	60/60 (100%)	1.64	21 (35%) 1 1	44, 102, 136, 160	0
15	O	88/88 (100%)	0.63	8 (9%) 15 16	17, 63, 122, 167	0
16	P	83/88 (94%)	0.73	10 (12%) 9 12	21, 56, 95, 122	0
17	Q	104/104 (100%)	0.66	8 (7%) 19 18	13, 56, 119, 198	0
18	R	73/88 (82%)	0.83	6 (8%) 17 17	35, 82, 143, 191	0
19	S	80/92 (86%)	0.83	9 (11%) 10 13	73, 124, 155, 197	0
20	T	99/106 (93%)	1.00	15 (15%) 5 8	38, 80, 118, 156	0
21	V	24/26 (92%)	2.27	9 (37%) 1 1	51, 88, 137, 141	0
22	Y	219/222 (98%)	0.75	23 (10%) 11 14	64, 119, 160, 196	0
All	All	4122/4263 (96%)	0.64	397 (9%) 13 15	11, 82, 153, 260	0

The worst 5 of 397 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	M	124	PRO	9.3
1	A	1492	A	8.3
14	N	22	THR	8.1
2	B	133	LYS	6.7
11	K	127	LYS	6.4

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 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($\text{\AA}^2$)	Q<0.9
23	MG	A	1677	1/1	-0.02	0.56	63,63,63,63	0
23	MG	A	1617	1/1	0.29	0.34	76,76,76,76	0
23	MG	A	1665	1/1	0.31	0.40	107,107,107,107	0
23	MG	A	1631	1/1	0.33	0.26	46,46,46,46	0
23	MG	A	1686	1/1	0.36	0.27	62,62,62,62	0
23	MG	A	1689	1/1	0.36	0.26	58,58,58,58	0
23	MG	A	1601	1/1	0.38	0.23	42,42,42,42	0
23	MG	A	1629	1/1	0.41	1.25	70,70,70,70	0
23	MG	A	1667	1/1	0.42	0.20	76,76,76,76	0
23	MG	A	1614	1/1	0.42	0.24	59,59,59,59	0
23	MG	B	301	1/1	0.43	0.15	59,59,59,59	0
23	MG	A	1656	1/1	0.44	0.28	33,33,33,33	0
23	MG	A	1644	1/1	0.46	0.26	54,54,54,54	0
23	MG	A	1624	1/1	0.46	0.67	70,70,70,70	0
23	MG	N	102	1/1	0.48	0.51	24,24,24,24	0
23	MG	A	1612	1/1	0.49	0.24	46,46,46,46	0
23	MG	A	1628	1/1	0.51	0.37	54,54,54,54	0
23	MG	A	1695	1/1	0.52	0.35	52,52,52,52	0
23	MG	A	1647	1/1	0.54	0.49	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	MG	A	1613	1/1	0.54	0.31	63,63,63,63	0
23	MG	A	1699	1/1	0.56	0.45	43,43,43,43	0
23	MG	A	1646	1/1	0.57	0.25	18,18,18,18	0
23	MG	A	1621	1/1	0.58	0.44	59,59,59,59	0
23	MG	A	1661	1/1	0.61	0.18	93,93,93,93	0
23	MG	A	1607	1/1	0.62	0.13	61,61,61,61	0
23	MG	A	1606	1/1	0.66	0.31	37,37,37,37	0
23	MG	A	1616	1/1	0.66	0.36	19,19,19,19	0
23	MG	A	1662	1/1	0.67	0.29	67,67,67,67	0
23	MG	A	1669	1/1	0.67	0.30	33,33,33,33	0
23	MG	A	1645	1/1	0.67	0.32	12,12,12,12	0
23	MG	A	1611	1/1	0.69	0.80	57,57,57,57	0
23	MG	A	1703	1/1	0.69	0.91	70,70,70,70	0
23	MG	A	1653	1/1	0.69	0.33	11,11,11,11	0
23	MG	A	1626	1/1	0.69	0.72	70,70,70,70	0
23	MG	A	1680	1/1	0.70	0.40	22,22,22,22	0
23	MG	A	1712	1/1	0.71	0.22	36,36,36,36	0
23	MG	A	1604	1/1	0.71	0.66	70,70,70,70	0
23	MG	A	1704	1/1	0.71	0.22	29,29,29,29	0
23	MG	A	1716	1/1	0.72	0.19	42,42,42,42	0
23	MG	A	1627	1/1	0.72	0.39	52,52,52,52	0
23	MG	A	1620	1/1	0.72	0.42	15,15,15,15	0
23	MG	A	1600	1/1	0.73	0.15	63,63,63,63	0
23	MG	A	1705	1/1	0.73	0.29	16,16,16,16	0
23	MG	A	1682	1/1	0.74	0.30	36,36,36,36	0
23	MG	A	1655	1/1	0.74	0.13	47,47,47,47	0
23	MG	A	1666	1/1	0.74	0.15	26,26,26,26	0
23	MG	A	1643	1/1	0.74	0.34	10,10,10,10	0
23	MG	A	1625	1/1	0.76	0.39	0,0,0,0	0
23	MG	A	1637	1/1	0.76	0.74	70,70,70,70	0
23	MG	A	1652	1/1	0.77	0.47	42,42,42,42	0
23	MG	A	1648	1/1	0.77	0.25	4,4,4,4	0
23	MG	A	1700	1/1	0.78	0.31	10,10,10,10	0
23	MG	A	1650	1/1	0.78	0.81	57,57,57,57	0
23	MG	A	1685	1/1	0.78	0.35	36,36,36,36	0
23	MG	A	1674	1/1	0.78	0.17	8,8,8,8	0
23	MG	A	1609	1/1	0.80	0.27	33,33,33,33	0
23	MG	A	1690	1/1	0.81	0.56	33,33,33,33	0
23	MG	A	1711	1/1	0.81	0.21	9,9,9,9	0
23	MG	A	1630	1/1	0.81	0.35	7,7,7,7	0
23	MG	A	1615	1/1	0.82	0.54	27,27,27,27	0
23	MG	A	1673	1/1	0.82	0.33	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	MG	A	1707	1/1	0.82	0.68	42,42,42,42	0
23	MG	A	1688	1/1	0.82	0.32	28,28,28,28	0
23	MG	A	1708	1/1	0.83	0.17	21,21,21,21	0
23	MG	A	1681	1/1	0.83	0.29	41,41,41,41	0
23	MG	A	1608	1/1	0.84	0.11	56,56,56,56	0
23	MG	A	1622	1/1	0.84	0.27	29,29,29,29	0
23	MG	A	1694	1/1	0.84	0.27	14,14,14,14	0
23	MG	A	1633	1/1	0.84	0.27	27,27,27,27	0
23	MG	A	1649	1/1	0.85	0.29	15,15,15,15	0
23	MG	A	1610	1/1	0.85	0.21	63,63,63,63	0
23	MG	A	1687	1/1	0.85	0.30	17,17,17,17	0
23	MG	A	1632	1/1	0.85	0.23	27,27,27,27	0
23	MG	A	1671	1/1	0.86	0.43	10,10,10,10	0
23	MG	A	1636	1/1	0.86	0.26	1,1,1,1	0
23	MG	A	1692	1/1	0.86	0.18	23,23,23,23	0
23	MG	A	1683	1/1	0.86	0.24	38,38,38,38	0
23	MG	A	1657	1/1	0.86	0.33	0,0,0,0	0
23	MG	A	1696	1/1	0.86	0.41	27,27,27,27	0
23	MG	A	1603	1/1	0.86	0.28	36,36,36,36	0
23	MG	A	1678	1/1	0.86	0.33	27,27,27,27	0
23	MG	A	1651	1/1	0.86	0.28	8,8,8,8	0
23	MG	A	1634	1/1	0.87	0.28	3,3,3,3	0
23	MG	A	1679	1/1	0.87	0.23	27,27,27,27	0
23	MG	A	1710	1/1	0.87	0.29	20,20,20,20	0
23	MG	A	1663	1/1	0.87	0.26	16,16,16,16	0
23	MG	A	1670	1/1	0.88	0.18	34,34,34,34	0
23	MG	A	1676	1/1	0.88	0.28	5,5,5,5	0
23	MG	A	1642	1/1	0.88	0.41	33,33,33,33	0
23	MG	A	1640	1/1	0.88	0.24	33,33,33,33	0
23	MG	A	1641	1/1	0.89	0.26	0,0,0,0	0
23	MG	A	1697	1/1	0.89	0.39	38,38,38,38	0
23	MG	E	201	1/1	0.89	0.44	21,21,21,21	0
23	MG	A	1715	1/1	0.89	0.26	9,9,9,9	0
23	MG	A	1658	1/1	0.90	0.27	40,40,40,40	0
23	MG	A	1635	1/1	0.90	0.39	25,25,25,25	0
25	SFG	Y	301	27/27	0.90	0.17	110,110,110,110	0
23	MG	A	1668	1/1	0.91	0.38	15,15,15,15	0
23	MG	A	1701	1/1	0.91	0.22	6,6,6,6	0
23	MG	A	1713	1/1	0.91	0.21	39,39,39,39	0
23	MG	A	1639	1/1	0.92	0.21	15,15,15,15	0
23	MG	A	1691	1/1	0.92	0.15	2,2,2,2	0
23	MG	A	1702	1/1	0.92	0.24	32,32,32,32	0

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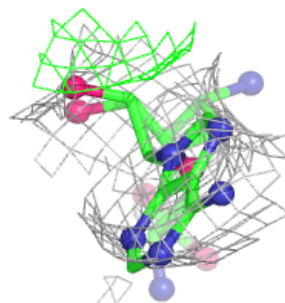
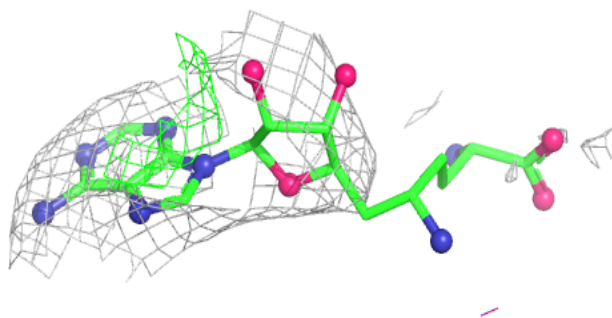
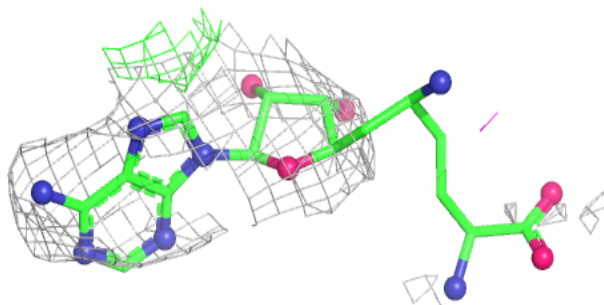
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	MG	A	1654	1/1	0.93	0.34	16,16,16,16	0
23	MG	A	1693	1/1	0.93	0.59	18,18,18,18	0
23	MG	A	1638	1/1	0.93	0.14	47,47,47,47	0
23	MG	A	1714	1/1	0.93	0.40	19,19,19,19	0
23	MG	A	1664	1/1	0.93	0.23	7,7,7,7	0
23	MG	A	1602	1/1	0.94	0.58	22,22,22,22	0
23	MG	A	1698	1/1	0.94	0.28	23,23,23,23	0
23	MG	A	1709	1/1	0.95	0.29	34,34,34,34	0
23	MG	A	1684	1/1	0.95	0.37	17,17,17,17	0
23	MG	A	1619	1/1	0.95	0.13	40,40,40,40	0
23	MG	A	1675	1/1	0.96	0.24	43,43,43,43	0
23	MG	A	1660	1/1	0.96	0.18	4,4,4,4	0
23	MG	A	1618	1/1	0.96	0.92	69,69,69,69	0
23	MG	A	1672	1/1	0.97	0.08	15,15,15,15	0
23	MG	A	1706	1/1	0.97	0.16	30,30,30,30	0
23	MG	A	1623	1/1	0.97	0.37	30,30,30,30	0
23	MG	A	1605	1/1	0.97	0.31	8,8,8,8	0
23	MG	A	1659	1/1	0.98	0.10	12,12,12,12	0
24	ZN	N	101	1/1	0.99	0.04	108,108,108,108	0
24	ZN	D	301	1/1	0.99	0.25	34,34,34,34	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 SFG Y 301:

$2mF_o - DF_c$ (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.