



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 04:12 PM UTC

PDB ID : 5IWA / pdb_00005iwa
Title : Crystal structure of the 30S ribosomal subunit from *Thermus thermophilus* in complex with the GE81112 peptide antibiotic
Authors : Schedlbauer, A.; Kaminishi, T.; Ochoa-Lizarralde, B.; Chieko, N.; Masahito, K.; Takemoto, C.; Yokoyama, S.; Connell, S.R.; Fucini, P.
Deposited on : 2016-03-22
Resolution : 3.50 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

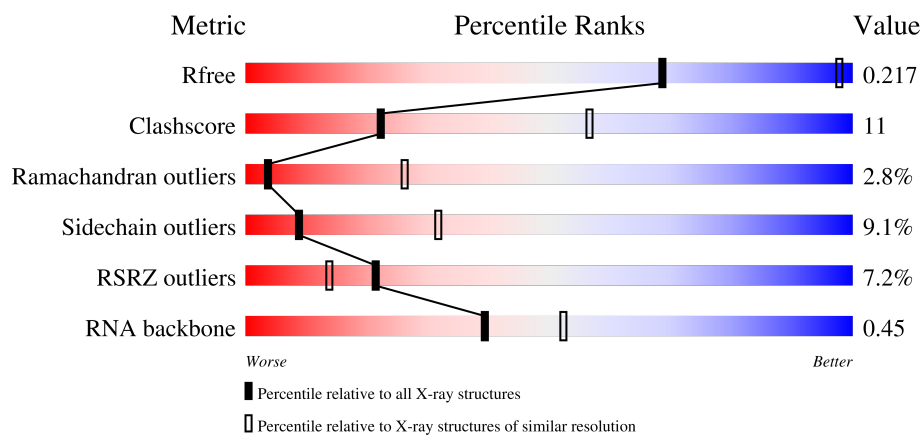
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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.



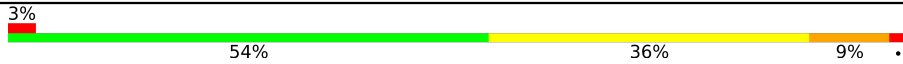
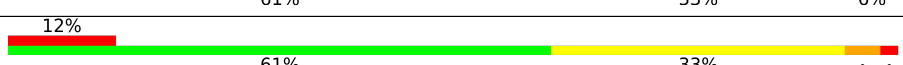
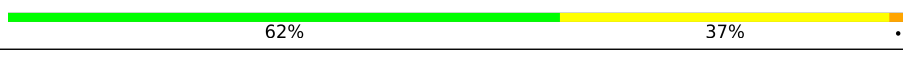
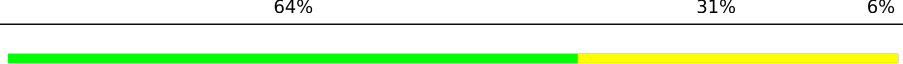
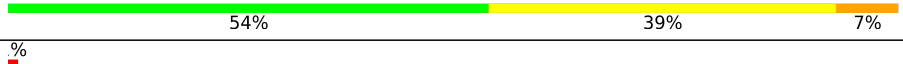
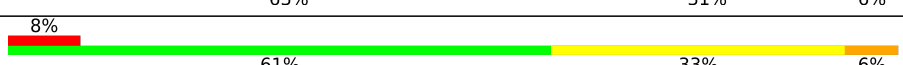
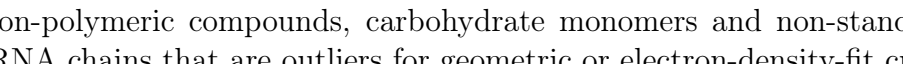
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)
RNA backbone	3983	1010 (3.98-3.02)

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	B	226	4% 59% 36% .
2	C	206	% 63% 33% .
3	D	208	5% 60% 34% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	E	157	
5	F	101	
6	G	155	
7	H	138	
8	I	127	
9	J	99	
10	K	115	
11	L	124	
12	M	125	
13	N	60	
14	O	88	
15	P	85	
16	Q	104	
17	R	71	
18	S	83	
19	T	103	
20	V	24	
21	A	1509	

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
22	MG	A	3438	-	-	-	X
22	MG	A	3453	-	-	-	X
22	MG	A	3483	-	-	-	X
23	ZN	N	101	-	-	X	-

2 Entry composition [i](#)

There are 24 unique types of molecules in this entry. The entry contains 52089 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 protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	225	Total	C	N	O	S	0	0	0
			1837	1171	331	330	5			

- Molecule 2 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	206	Total	C	N	O	S	0	0	0
			1613	1016	314	282	1			

- Molecule 3 is a protein called 30S ribosomal protein S4.

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

- Molecule 4 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	157	Total	C	N	O	S	0	0	0
			1199	754	228	213	4			

- Molecule 5 is a protein called 30S ribosomal protein S6.

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

- Molecule 6 is a protein called 30S ribosomal protein S7.

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

- Molecule 7 is a protein called 30S ribosomal protein S8.

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

- Molecule 8 is a protein called 30S ribosomal protein S9.

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

- Molecule 9 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	99	Total	C	N	O	S	0	0	0
			802	504	157	140	1			

- Molecule 10 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	K	115	Total	C	N	O	S	0	0	0
			854	531	160	160	3			

- Molecule 11 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	124	Total	C	N	O	S	0	0	0
			971	611	195	164	1			

- Molecule 12 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	125	Total	C	N	O	S	0	0	0
			987	611	203	171	2			

- Molecule 13 is a protein called 30S ribosomal protein S14 type Z.

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

- Molecule 14 is a protein called 30S ribosomal protein S15.

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

- Molecule 15 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	P	85	Total	C	N	O	S	0	0	0
			717	452	144	120	1			

- Molecule 16 is a protein called 30S ribosomal protein S17.

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

- Molecule 17 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	R	71	Total	C	N	O	S	0	0	0
			585	373	116	96				

- Molecule 18 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	S	83	Total	C	N	O	S	0	0	0
			666	424	124	116	2			

- Molecule 19 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	T	103	Total	C	N	O	S	0	0	0
			797	493	169	133	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	V	24	Total	C	N	O	S	0	0	0
			209	128	50	31				

- Molecule 21 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	A	1509	Total	C	N	O	P	0	7	0
			32589	14507	6043	10524	1515			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	A	-	expression tag	GB 55771382
A	2	A	-	expression tag	GB 55771382
A	3	A	-	expression tag	GB 55771382

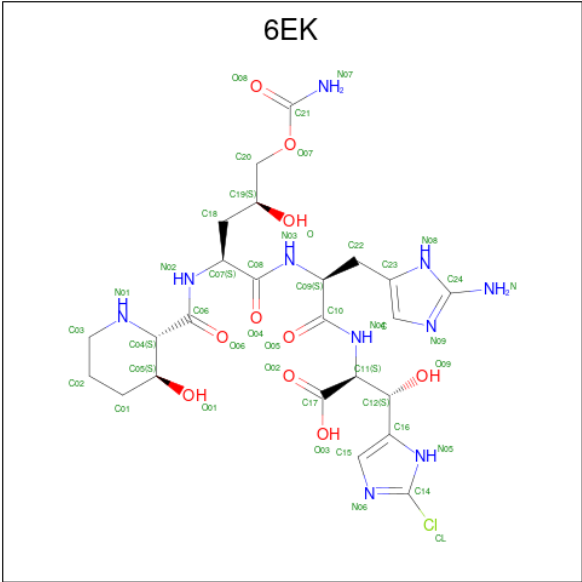
- Molecule 22 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	B	1	Total	Mg	0	0
			1	1		
22	E	1	Total	Mg	0	0
			1	1		
22	H	1	Total	Mg	0	0
			1	1		
22	K	1	Total	Mg	0	0
			1	1		
22	O	1	Total	Mg	0	0
			1	1		
22	S	1	Total	Mg	0	0
			1	1		
22	A	198	Total	Mg	0	0
			198	198		

- Molecule 23 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 24 is (2S,3S)-2-{[(2S)-3-(2-amino-1H-imidazol-5-yl)-2-{[(2S,4S)-5-(carbamoyloxy)-4-hydroxy-2-({[(2S,3S)-3-hydroxypiperidin-2-yl]carbonyl}amino)pentanoyl]amino}propanoyl]amino}-3-(2-chloro-1H-imidazol-5-yl)-3-hydroxypropanoic acid (CCD ID: 6EK) (formula: C₂₄H₃₅ClN₁₀O₁₀).

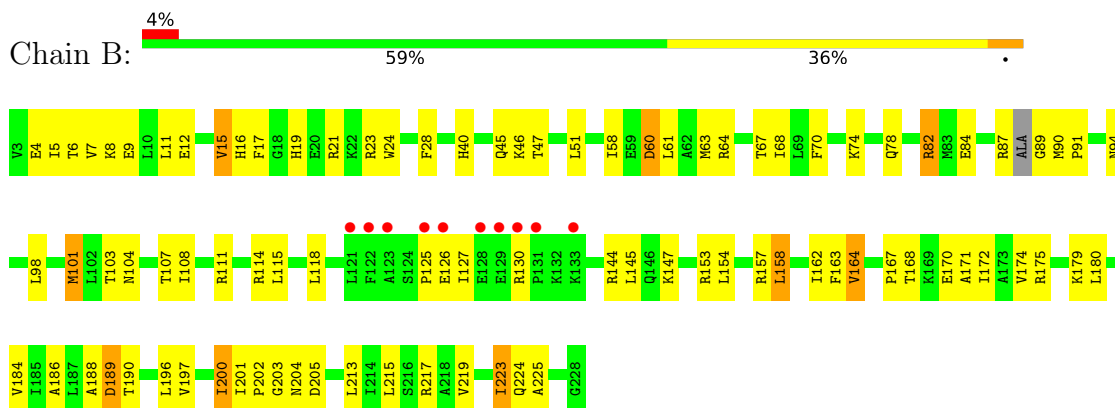


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	M	1	Total	C	Cl	N	O	0	0
			45	24	1	10	10		

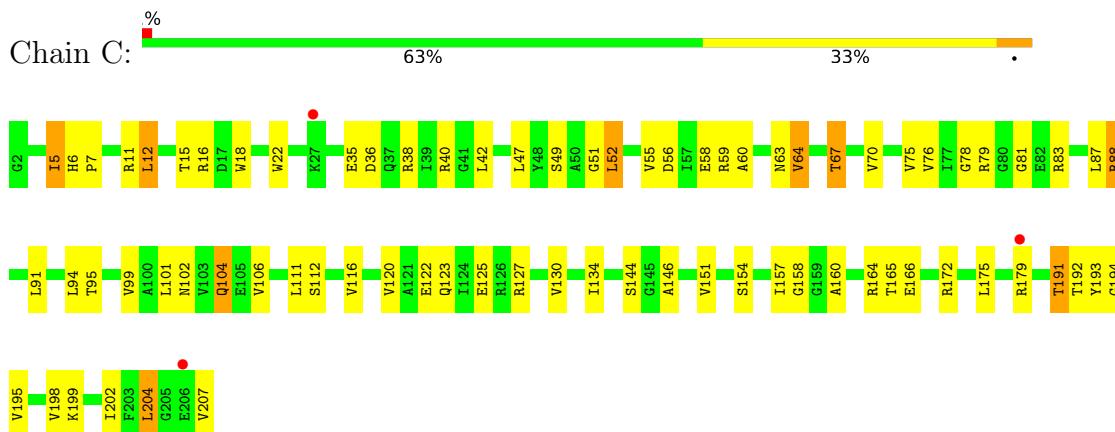
3 Residue-property plots [i](#)

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.

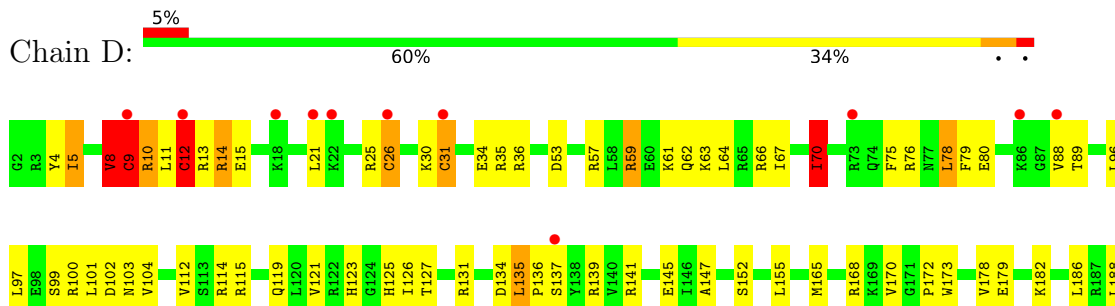
• Molecule 1: 30S ribosomal protein S2

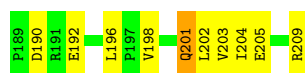


• Molecule 2: 30S ribosomal protein S3



• Molecule 3: 30S ribosomal protein S4





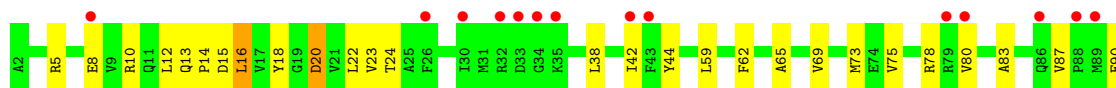
• Molecule 4: 30S ribosomal protein S5



• Molecule 5: 30S ribosomal protein S6



• Molecule 6: 30S ribosomal protein S7

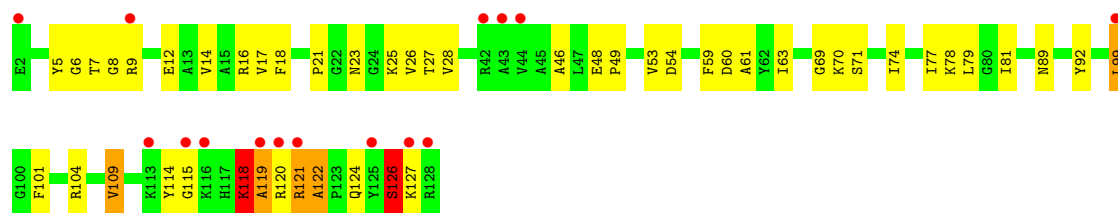


• Molecule 7: 30S ribosomal protein S8

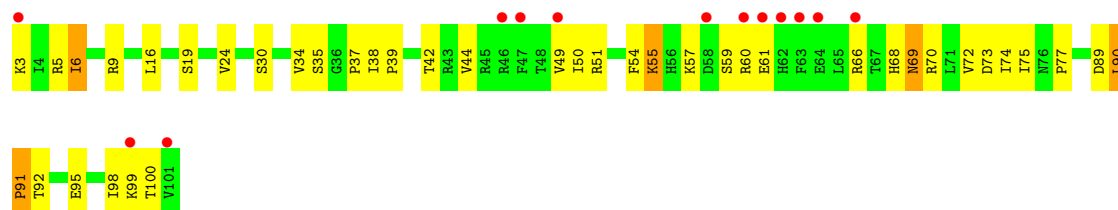


• Molecule 8: 30S ribosomal protein S9

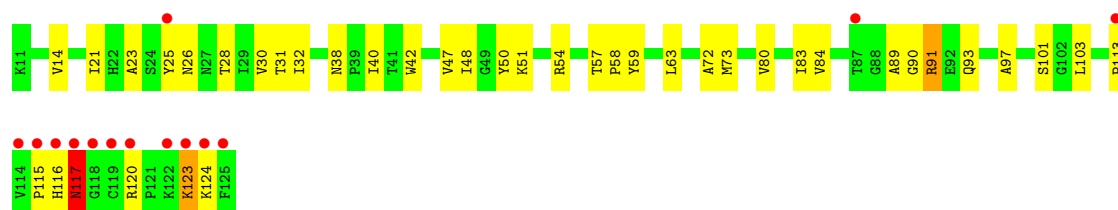




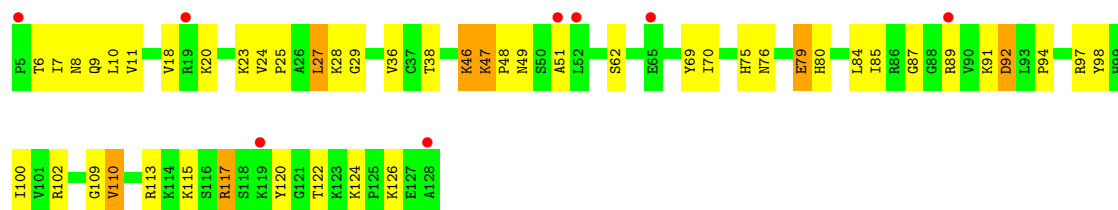
• Molecule 9: 30S ribosomal protein S10



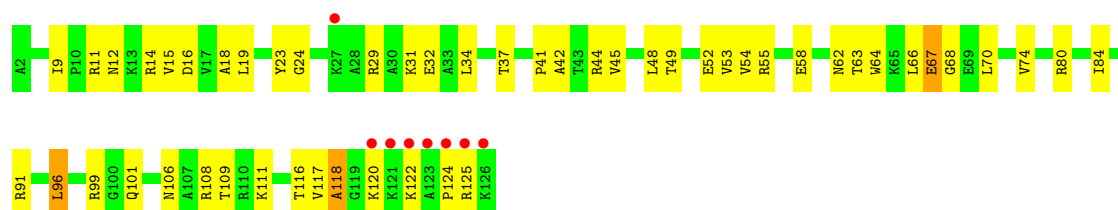
• Molecule 10: 30S ribosomal protein S11



• Molecule 11: 30S ribosomal protein S12



• Molecule 12: 30S ribosomal protein S13



- Molecule 13: 30S ribosomal protein S14 type Z

Chain N:  62% 37% .



- Molecule 14: 30S ribosomal protein S15

Chain O:  64% 31% 6%



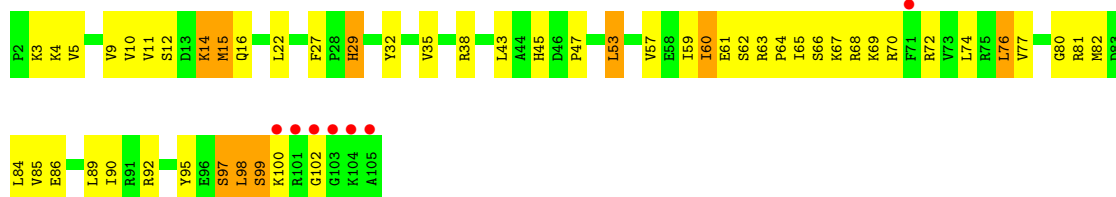
- Molecule 15: 30S ribosomal protein S16

Chain P:  64% 36%



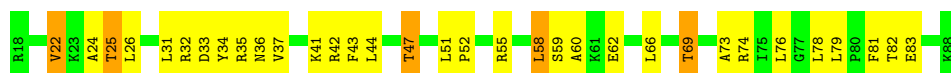
- Molecule 16: 30S ribosomal protein S17

Chain Q:  7% 50% 41% 9%



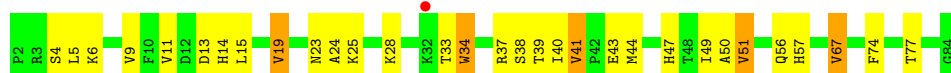
- Molecule 17: 30S ribosomal protein S18

Chain R:  54% 39% 7%



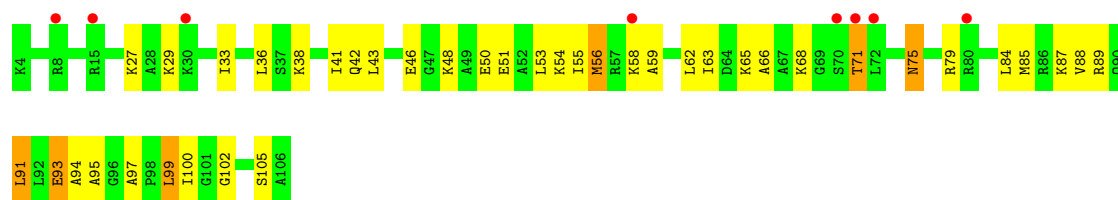
- Molecule 18: 30S ribosomal protein S19

Chain S:  63% 31% 6%

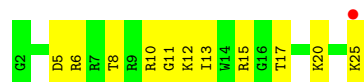


- Molecule 19: 30S ribosomal protein S20

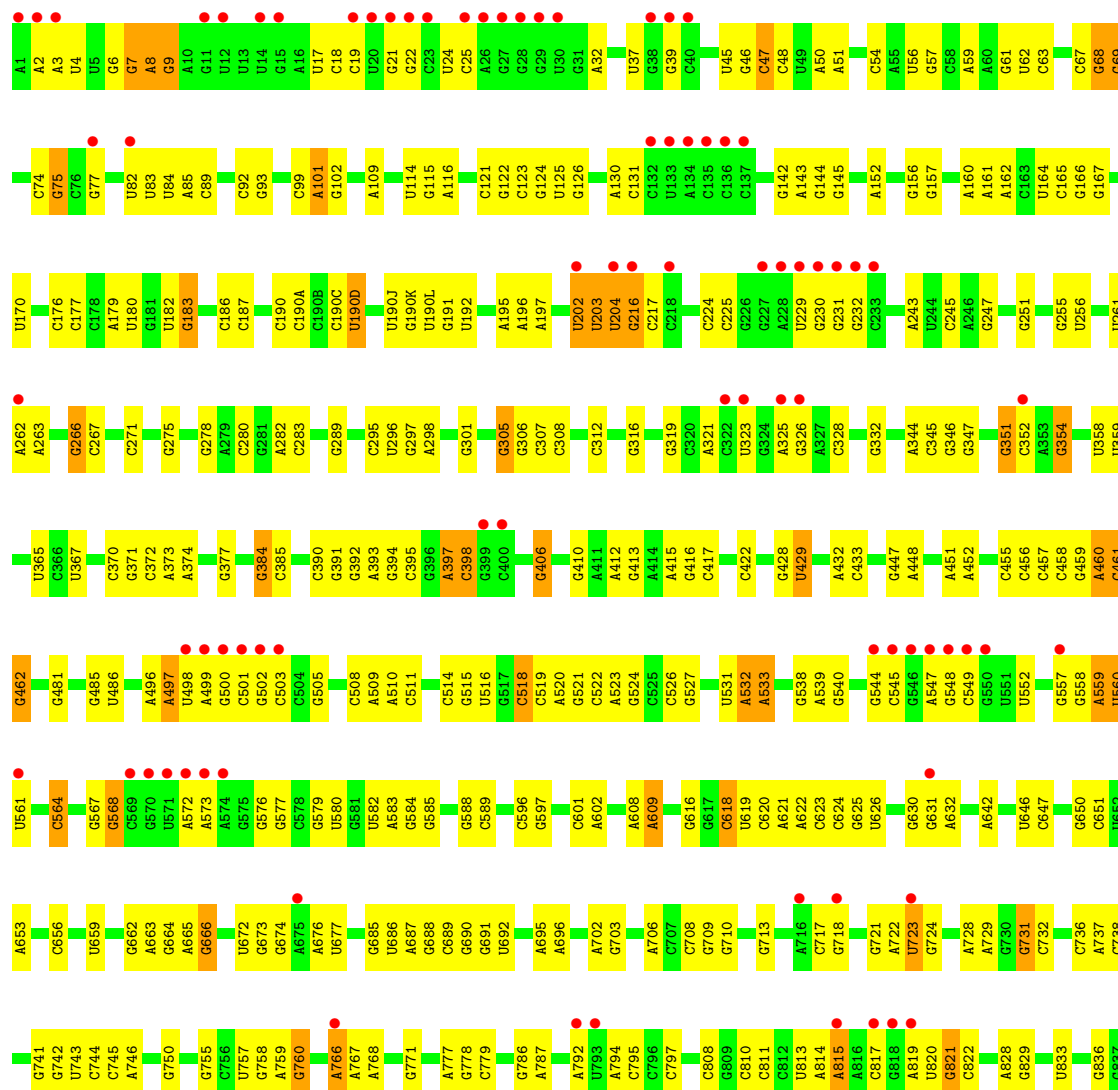
Chain T:  8% 61% 33% 6%

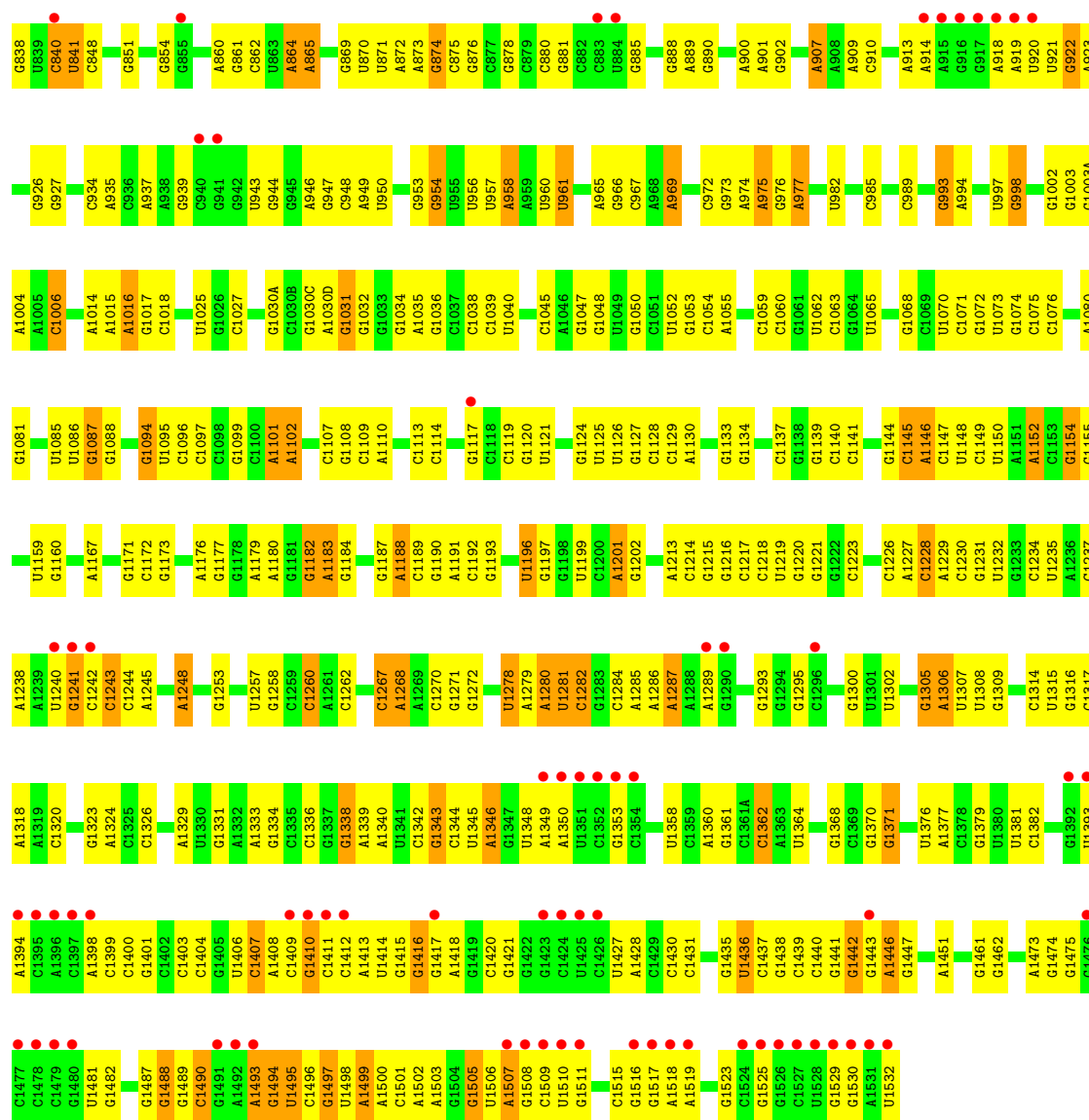


- Molecule 20: 30S ribosomal protein Thx



- Molecule 21: 16S ribosomal RNA





4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	413.14Å 413.14Å 173.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	80.03 – 3.50 80.03 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (80.03-3.50) 99.8 (80.03-3.50)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 3.49Å)	Xtriage
Refinement program	PHENIX 1.7.3 _928	Depositor
R, R_{free}	0.166 , 0.218 0.169 , 0.217	Depositor DCC
R_{free} test set	9369 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	138.9	Xtriage
Anisotropy	0.232	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 109.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	52089	wwPDB-VP
Average B, all atoms (Å ²)	146.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% 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: 6EK, MG, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	B	0.64	0/1868	1.06	4/2512 (0.2%)
2	C	0.65	0/1637	1.04	4/2205 (0.2%)
3	D	0.74	0/1733	1.21	11/2318 (0.5%)
4	E	0.87	0/1216	1.34	13/1636 (0.8%)
5	F	0.58	0/856	1.05	2/1154 (0.2%)
6	G	0.57	0/1276	0.96	0/1709
7	H	0.79	0/1136	1.28	12/1527 (0.8%)
8	I	0.60	0/1029	1.09	8/1379 (0.6%)
9	J	0.62	0/815	1.01	2/1095 (0.2%)
10	K	0.63	0/869	1.12	7/1173 (0.6%)
11	L	0.69	0/987	1.13	4/1320 (0.3%)
12	M	0.60	0/998	1.07	3/1336 (0.2%)
13	N	0.61	0/501	1.17	5/664 (0.8%)
14	O	0.63	0/745	1.04	1/992 (0.1%)
15	P	0.69	0/733	1.04	3/984 (0.3%)
16	Q	0.68	0/870	1.14	6/1159 (0.5%)
17	R	0.66	0/590	1.04	0/782
18	S	0.52	0/681	0.95	2/915 (0.2%)
19	T	0.56	0/800	1.08	3/1052 (0.3%)
20	V	0.58	0/213	1.02	1/277 (0.4%)
21	A	0.41	0/36483	0.48	0/56943
All	All	0.51	0/56036	0.74	91/83132 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	D	0	1
7	H	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
11	L	0	1
All	All	0	3

There are no bond length outliers.

The worst 5 of 91 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	51	VAL	CB-CA-C	-10.69	103.02	114.35
7	H	71	GLY	CA-C-N	-10.33	109.42	120.47
7	H	71	GLY	C-N-CA	-10.33	109.42	120.47
3	D	31	CYS	N-CA-C	-9.03	97.71	110.35
3	D	9	CYS	N-CA-C	-8.28	93.17	110.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	11	LEU	Peptide
7	H	90	GLY	Peptide
11	L	46	LYS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1837	0	1888	57	0
2	C	1613	0	1677	39	0
3	D	1703	0	1764	52	0
4	E	1199	0	1251	50	0
5	F	843	0	857	27	0
6	G	1257	0	1296	31	0
7	H	1116	0	1177	27	0
8	I	1010	0	1037	30	0
9	J	802	0	849	27	0
10	K	854	0	868	24	0
11	L	971	0	1057	28	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	M	987	0	1050	33	0
13	N	492	0	530	15	0
14	O	734	0	771	21	0
15	P	717	0	738	18	0
16	Q	857	0	928	35	0
17	R	585	0	657	26	0
18	S	666	0	686	20	0
19	T	797	0	907	25	0
20	V	209	0	221	6	0
21	A	32589	0	16447	443	0
22	A	198	0	0	0	0
22	B	1	0	0	0	0
22	E	1	0	0	0	0
22	H	1	0	0	0	0
22	K	1	0	0	0	0
22	O	1	0	0	0	0
22	S	1	0	0	0	0
23	D	1	0	0	0	0
23	N	1	0	0	2	0
24	M	45	0	0	0	0
All	All	52089	0	36656	928	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 11.

The worst 5 of 928 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:J:61:GLU:OE1	13:N:45:ARG:NH1	2.00	0.93
21:A:664:G:H22	21:A:741:G:H1	1.21	0.88
6:G:94:ARG:NH1	21:A:1377:A:OP2	2.10	0.85
10:K:57:THR:HG22	10:K:59:TYR:H	1.40	0.84
8:I:16:ARG:NH1	21:A:1147:C:O2	2.11	0.84

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	
1	B	221/226 (98%)	184 (83%)	32 (14%)	5 (2%)	5	30
2	C	204/206 (99%)	176 (86%)	23 (11%)	5 (2%)	4	28
3	D	206/208 (99%)	185 (90%)	18 (9%)	3 (2%)	8	37
4	E	155/157 (99%)	132 (85%)	17 (11%)	6 (4%)	2	20
5	F	99/101 (98%)	87 (88%)	12 (12%)	0	100	100
6	G	153/155 (99%)	127 (83%)	22 (14%)	4 (3%)	4	27
7	H	136/138 (99%)	118 (87%)	15 (11%)	3 (2%)	5	30
8	I	125/127 (98%)	102 (82%)	18 (14%)	5 (4%)	2	19
9	J	97/99 (98%)	77 (79%)	14 (14%)	6 (6%)	1	12
10	K	113/115 (98%)	98 (87%)	14 (12%)	1 (1%)	14	47
11	L	122/124 (98%)	104 (85%)	16 (13%)	2 (2%)	7	36
12	M	123/125 (98%)	101 (82%)	16 (13%)	6 (5%)	1	16
13	N	58/60 (97%)	49 (84%)	7 (12%)	2 (3%)	3	23
14	O	86/88 (98%)	69 (80%)	11 (13%)	6 (7%)	1	10
15	P	83/85 (98%)	71 (86%)	11 (13%)	1 (1%)	10	41
16	Q	102/104 (98%)	84 (82%)	11 (11%)	7 (7%)	1	10
17	R	69/71 (97%)	59 (86%)	8 (12%)	2 (3%)	3	26
18	S	81/83 (98%)	69 (85%)	11 (14%)	1 (1%)	10	41
19	T	101/103 (98%)	86 (85%)	13 (13%)	2 (2%)	6	32
20	V	22/24 (92%)	20 (91%)	2 (9%)	0	100	100
All	All	2356/2399 (98%)	1998 (85%)	291 (12%)	67 (3%)	4	26

5 of 67 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	78	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	70	ILE
4	E	146	ALA
4	E	154	GLY
4	E	156	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	
1	B	195/195 (100%)	179 (92%)	16 (8%)	10	34
2	C	160/160 (100%)	139 (87%)	21 (13%)	4	20
3	D	180/180 (100%)	161 (89%)	19 (11%)	6	27
4	E	119/119 (100%)	104 (87%)	15 (13%)	4	21
5	F	90/90 (100%)	78 (87%)	12 (13%)	4	20
6	G	126/126 (100%)	119 (94%)	7 (6%)	19	46
7	H	119/119 (100%)	108 (91%)	11 (9%)	8	32
8	I	98/98 (100%)	90 (92%)	8 (8%)	10	34
9	J	89/89 (100%)	80 (90%)	9 (10%)	7	28
10	K	87/87 (100%)	81 (93%)	6 (7%)	14	39
11	L	104/104 (100%)	92 (88%)	12 (12%)	5	24
12	M	98/100 (98%)	93 (95%)	5 (5%)	21	48
13	N	49/49 (100%)	45 (92%)	4 (8%)	10	34
14	O	79/79 (100%)	76 (96%)	3 (4%)	29	55
15	P	73/73 (100%)	66 (90%)	7 (10%)	8	30
16	Q	96/96 (100%)	88 (92%)	8 (8%)	10	34
17	R	62/62 (100%)	57 (92%)	5 (8%)	11	35
18	S	72/72 (100%)	66 (92%)	6 (8%)	10	34
19	T	80/80 (100%)	74 (92%)	6 (8%)	12	37
20	V	19/19 (100%)	17 (90%)	2 (10%)	6	27

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1995/1997 (100%)	1813 (91%)	182 (9%)	9 32

5 of 182 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	J	92	THR
13	N	22	THR
10	K	47	VAL
11	L	62	SER
15	P	25	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
14	O	62	GLN
19	T	75	ASN
18	S	47	HIS
6	G	13	GLN
10	K	117	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	A	1501/1509 (99%)	282 (18%)	11 (0%)

5 of 282 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	A	2	A
21	A	3	A
21	A	4	U
21	A	6	G
21	A	7	G

5 of 11 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
21	A	1145	C
21	A	1281	U
21	A	1417	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	A	1410	G
21	A	460	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 207 ligands modelled in this entry, 206 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	6EK	M	201	-	42,47,47	2.74	16 (38%)	48,65,65	2.13	14 (29%)

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	6EK	M	201	-	-	12/49/60/60	0/3/3/3

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	M	201	6EK	C21-N07	6.80	1.45	1.33
24	M	201	6EK	C10-N04	6.68	1.48	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	M	201	6EK	C08-N03	5.94	1.46	1.34
24	M	201	6EK	C06-N02	5.65	1.46	1.34
24	M	201	6EK	C24-N	5.23	1.46	1.34

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	M	201	6EK	O07-C21-N07	7.04	119.87	111.11
24	M	201	6EK	O08-C21-N07	-4.50	118.48	125.58
24	M	201	6EK	N08-C24-N09	-4.43	108.34	112.36
24	M	201	6EK	O07-C21-O08	-3.72	119.65	123.08
24	M	201	6EK	C20-O07-C21	3.26	120.84	116.26

There are no chirality outliers.

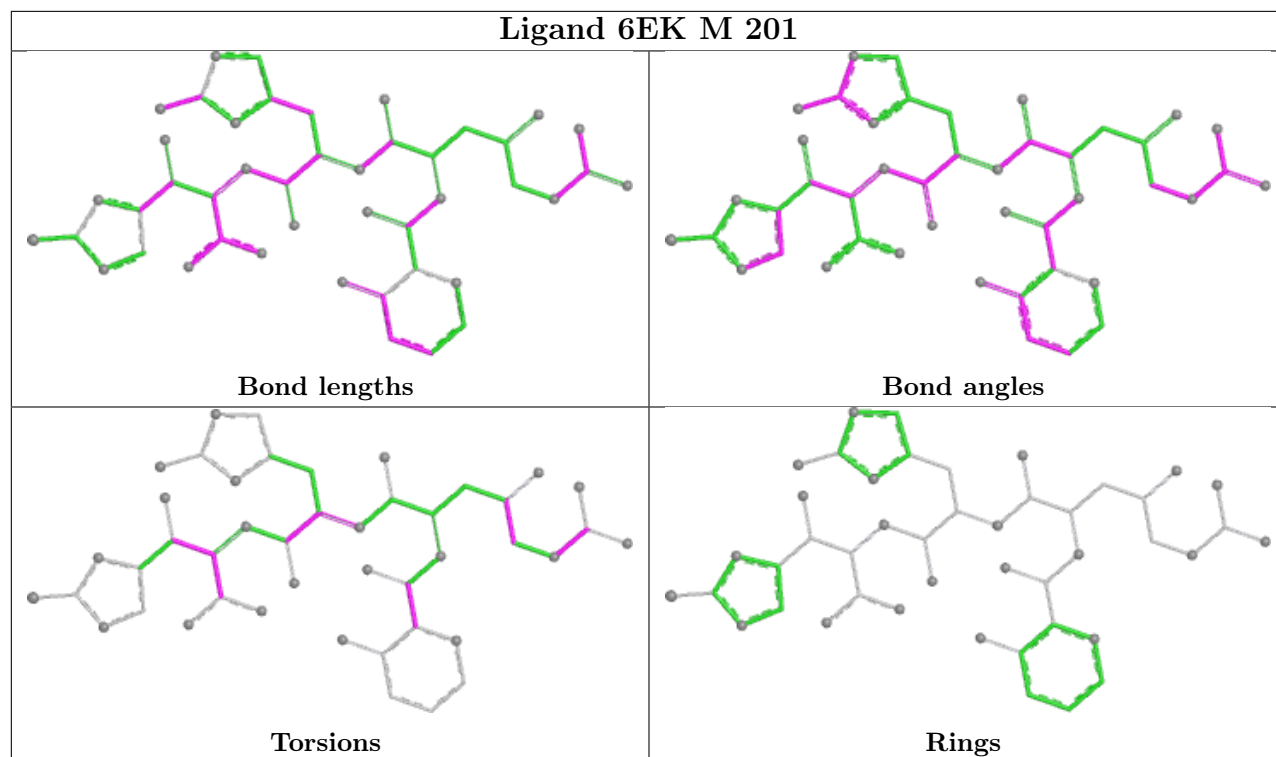
5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	M	201	6EK	N07-C21-O07-C20
24	M	201	6EK	O08-C21-O07-C20
24	M	201	6EK	N01-C04-C06-N02
24	M	201	6EK	N04-C11-C12-O09
24	M	201	6EK	C12-C11-C17-O02

There are no ring outliers.

No monomer is involved in short contacts.

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	B	225/226 (99%)	-0.30	10 (4%) 39 21	92, 135, 194, 222	0
2	C	206/206 (100%)	-0.33	3 (1%) 72 47	106, 140, 172, 207	0
3	D	208/208 (100%)	0.15	11 (5%) 32 18	92, 124, 157, 174	0
4	E	157/157 (100%)	-0.04	5 (3%) 50 29	84, 109, 158, 232	0
5	F	101/101 (100%)	-0.31	0 100 100	113, 158, 201, 242	0
6	G	155/155 (100%)	0.57	23 (14%) 5 5	128, 170, 207, 228	0
7	H	138/138 (100%)	-0.26	3 (2%) 62 37	83, 110, 139, 192	0
8	I	127/127 (100%)	0.40	15 (11%) 9 6	110, 166, 204, 217	0
9	J	99/99 (100%)	0.51	13 (13%) 7 6	112, 168, 227, 242	0
10	K	115/115 (100%)	0.26	14 (12%) 8 6	118, 155, 183, 197	0
11	L	124/124 (100%)	0.34	8 (6%) 25 15	96, 133, 163, 224	0
12	M	125/125 (100%)	0.01	8 (6%) 25 15	128, 160, 190, 363	0
13	N	60/60 (100%)	-0.26	0 100 100	113, 134, 162, 175	0
14	O	88/88 (100%)	-0.46	0 100 100	107, 135, 169, 205	0
15	P	85/85 (100%)	-0.10	0 100 100	103, 129, 159, 215	0
16	Q	104/104 (100%)	0.27	7 (6%) 24 15	98, 133, 169, 247	0
17	R	71/71 (100%)	-0.41	0 100 100	106, 137, 201, 218	0
18	S	83/83 (100%)	0.09	1 (1%) 76 52	145, 168, 199, 215	0
19	T	103/103 (100%)	0.20	8 (7%) 19 12	130, 156, 198, 227	0
20	V	24/24 (100%)	0.36	1 (4%) 40 22	136, 149, 173, 177	0
21	A	1509/1509 (100%)	0.03	150 (9%) 13 8	64, 138, 216, 315	7 (0%)
All	All	3907/3908 (99%)	0.02	280 (7%) 21 14	64, 141, 204, 363	7 (0%)

The worst 5 of 280 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	G	33	ASP	8.2
10	K	117	ASN	7.6
21	A	136	C	7.4
6	G	106	GLN	7.0
21	A	793[A]	U	6.6

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
22	MG	A	3495	1/1	0.46	0.28	135,135,135,135	0
22	MG	A	3564	1/1	0.57	0.12	127,127,127,127	0
22	MG	A	3486	1/1	0.58	0.23	121,121,121,121	0
22	MG	A	3543	1/1	0.63	0.24	126,126,126,126	0
22	MG	A	3515	1/1	0.64	0.19	130,130,130,130	0
22	MG	A	3552	1/1	0.66	0.12	118,118,118,118	0
22	MG	A	3483	1/1	0.67	0.40	112,112,112,112	0
22	MG	A	3451	1/1	0.69	0.35	129,129,129,129	0
22	MG	A	3528	1/1	0.69	0.19	125,125,125,125	0
22	MG	A	3529	1/1	0.69	0.32	119,119,119,119	0
22	MG	A	3589	1/1	0.69	0.20	109,109,109,109	0
22	MG	A	3430	1/1	0.70	0.27	133,133,133,133	0
22	MG	A	3562	1/1	0.70	0.28	114,114,114,114	0
22	MG	A	3540	1/1	0.70	0.14	121,121,121,121	0
22	MG	A	3583	1/1	0.70	0.37	113,113,113,113	0
22	MG	A	3438	1/1	0.70	0.48	124,124,124,124	0
22	MG	A	3513	1/1	0.71	0.14	145,145,145,145	0
22	MG	A	3530	1/1	0.72	0.17	113,113,113,113	0
22	MG	A	3587	1/1	0.73	0.14	115,115,115,115	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	MG	A	3457	1/1	0.73	0.38	111,111,111,111	0
22	MG	A	3401	1/1	0.74	0.22	137,137,137,137	0
22	MG	A	3554	1/1	0.75	0.18	122,122,122,122	0
22	MG	A	3406	1/1	0.75	0.07	111,111,111,111	0
22	MG	A	3424	1/1	0.75	0.19	133,133,133,133	0
22	MG	A	3576	1/1	0.75	0.27	114,114,114,114	0
22	MG	A	3429	1/1	0.75	0.24	134,134,134,134	0
22	MG	A	3464	1/1	0.75	0.28	108,108,108,108	0
22	MG	S	101	1/1	0.75	0.30	118,118,118,118	0
22	MG	A	3412	1/1	0.76	0.32	122,122,122,122	0
22	MG	A	3474	1/1	0.76	0.23	92,92,92,92	0
22	MG	A	3481	1/1	0.76	0.30	103,103,103,103	0
22	MG	A	3510	1/1	0.77	0.32	101,101,101,101	0
22	MG	A	3550	1/1	0.78	0.34	123,123,123,123	0
22	MG	A	3425	1/1	0.78	0.29	106,106,106,106	0
22	MG	A	3416	1/1	0.78	0.31	125,125,125,125	0
22	MG	A	3465	1/1	0.79	0.24	136,136,136,136	0
22	MG	A	3442	1/1	0.79	0.19	101,101,101,101	0
22	MG	A	3476	1/1	0.79	0.32	111,111,111,111	0
22	MG	A	3427	1/1	0.79	0.22	112,112,112,112	0
22	MG	A	3405	1/1	0.79	0.08	125,125,125,125	0
22	MG	A	3439	1/1	0.79	0.24	114,114,114,114	0
22	MG	A	3477	1/1	0.80	0.66	94,94,94,94	0
22	MG	A	3453	1/1	0.80	0.48	110,110,110,110	0
22	MG	A	3582	1/1	0.81	0.10	111,111,111,111	0
22	MG	A	3531	1/1	0.81	0.59	135,135,135,135	0
22	MG	B	301	1/1	0.81	0.20	131,131,131,131	0
22	MG	O	101	1/1	0.81	0.45	92,92,92,92	0
22	MG	A	3404	1/1	0.82	0.26	105,105,105,105	0
22	MG	A	3432	1/1	0.82	0.21	101,101,101,101	0
22	MG	A	3595	1/1	0.82	0.64	127,127,127,127	0
22	MG	A	3571	1/1	0.83	0.31	108,108,108,108	0
22	MG	A	3573	1/1	0.83	0.42	99,99,99,99	0
22	MG	A	3418	1/1	0.83	0.21	124,124,124,124	0
22	MG	A	3541	1/1	0.83	0.23	108,108,108,108	0
22	MG	A	3435	1/1	0.84	0.43	132,132,132,132	0
22	MG	A	3469	1/1	0.84	0.21	83,83,83,83	0
22	MG	A	3551	1/1	0.84	0.25	94,94,94,94	0
22	MG	A	3512	1/1	0.85	0.21	122,122,122,122	0
22	MG	A	3506	1/1	0.85	0.07	128,128,128,128	0
22	MG	A	3502	1/1	0.85	0.26	100,100,100,100	0
22	MG	A	3594	1/1	0.85	0.20	115,115,115,115	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	MG	A	3511	1/1	0.85	0.28	76,76,76,76	0
22	MG	A	3561	1/1	0.86	0.29	98,98,98,98	0
22	MG	A	3407	1/1	0.86	0.19	96,96,96,96	0
22	MG	A	3484	1/1	0.86	0.37	91,91,91,91	0
22	MG	A	3500	1/1	0.86	0.36	108,108,108,108	0
22	MG	A	3598	1/1	0.86	0.70	123,123,123,123	0
22	MG	A	3534	1/1	0.87	0.23	112,112,112,112	0
22	MG	A	3473	1/1	0.87	0.30	89,89,89,89	0
22	MG	A	3485	1/1	0.87	0.58	96,96,96,96	0
22	MG	A	3575	1/1	0.87	0.20	138,138,138,138	0
22	MG	A	3431	1/1	0.87	0.17	111,111,111,111	0
22	MG	A	3426	1/1	0.87	0.15	98,98,98,98	0
22	MG	A	3563	1/1	0.88	0.07	132,132,132,132	0
22	MG	A	3468	1/1	0.88	0.06	128,128,128,128	0
22	MG	A	3440	1/1	0.88	0.15	124,124,124,124	0
22	MG	A	3556	1/1	0.88	0.09	84,84,84,84	0
22	MG	A	3590	1/1	0.88	0.14	111,111,111,111	0
22	MG	A	3538	1/1	0.88	0.27	95,95,95,95	0
22	MG	A	3516	1/1	0.88	0.11	95,95,95,95	0
22	MG	A	3577	1/1	0.88	0.15	88,88,88,88	0
24	6EK	M	201	45/45	0.88	0.18	180,269,292,301	0
22	MG	A	3544	1/1	0.89	0.10	119,119,119,119	0
22	MG	A	3574	1/1	0.89	0.12	100,100,100,100	0
22	MG	A	3501	1/1	0.89	0.34	83,83,83,83	0
22	MG	A	3452	1/1	0.89	0.20	93,93,93,93	0
22	MG	A	3514	1/1	0.89	0.18	104,104,104,104	0
22	MG	A	3578	1/1	0.89	0.22	108,108,108,108	0
22	MG	A	3533	1/1	0.89	0.09	118,118,118,118	0
22	MG	A	3491	1/1	0.89	0.31	104,104,104,104	0
22	MG	A	3479	1/1	0.89	0.24	94,94,94,94	0
22	MG	A	3539	1/1	0.89	0.08	108,108,108,108	0
22	MG	A	3518	1/1	0.89	0.16	115,115,115,115	0
22	MG	A	3526	1/1	0.89	0.13	110,110,110,110	0
22	MG	A	3567	1/1	0.89	0.09	103,103,103,103	0
22	MG	A	3597	1/1	0.89	0.19	128,128,128,128	0
22	MG	A	3569	1/1	0.89	0.11	105,105,105,105	0
22	MG	A	3414	1/1	0.89	0.26	92,92,92,92	0
22	MG	A	3467	1/1	0.90	0.45	85,85,85,85	0
22	MG	A	3527	1/1	0.90	0.28	98,98,98,98	0
22	MG	A	3592	1/1	0.90	0.14	114,114,114,114	0
22	MG	A	3579	1/1	0.90	0.15	94,94,94,94	0
22	MG	A	3456	1/1	0.90	0.23	95,95,95,95	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	MG	A	3517	1/1	0.90	0.19	82,82,82,82	0
22	MG	A	3408	1/1	0.90	0.18	108,108,108,108	0
22	MG	A	3588	1/1	0.90	0.11	105,105,105,105	0
22	MG	A	3570	1/1	0.91	0.18	102,102,102,102	0
22	MG	A	3524	1/1	0.91	0.10	85,85,85,85	0
22	MG	A	3411	1/1	0.91	0.32	117,117,117,117	0
22	MG	A	3403	1/1	0.91	0.33	83,83,83,83	0
22	MG	A	3410	1/1	0.91	0.30	76,76,76,76	0
22	MG	A	3449	1/1	0.91	0.21	114,114,114,114	0
22	MG	A	3489	1/1	0.91	0.16	111,111,111,111	0
22	MG	A	3482	1/1	0.91	0.32	92,92,92,92	0
22	MG	A	3532	1/1	0.91	0.06	119,119,119,119	0
22	MG	A	3581	1/1	0.91	0.26	107,107,107,107	0
22	MG	A	3492	1/1	0.91	0.38	97,97,97,97	0
22	MG	A	3585	1/1	0.92	0.23	114,114,114,114	0
22	MG	A	3586	1/1	0.92	0.43	112,112,112,112	0
22	MG	A	3523	1/1	0.92	0.10	85,85,85,85	0
22	MG	A	3422	1/1	0.92	0.19	89,89,89,89	0
22	MG	A	3499	1/1	0.92	0.10	107,107,107,107	0
22	MG	A	3417	1/1	0.92	0.28	85,85,85,85	0
22	MG	A	3448	1/1	0.92	0.22	97,97,97,97	0
22	MG	A	3409	1/1	0.92	0.38	83,83,83,83	0
22	MG	A	3493	1/1	0.92	0.26	92,92,92,92	0
22	MG	A	3507	1/1	0.92	0.34	105,105,105,105	0
22	MG	A	3508	1/1	0.92	0.21	107,107,107,107	0
22	MG	A	3509	1/1	0.92	0.22	100,100,100,100	0
22	MG	A	3450	1/1	0.93	0.29	89,89,89,89	0
22	MG	A	3535	1/1	0.93	0.23	68,68,68,68	0
22	MG	A	3488	1/1	0.93	0.25	115,115,115,115	0
22	MG	A	3494	1/1	0.93	0.32	94,94,94,94	0
22	MG	A	3557	1/1	0.93	0.06	103,103,103,103	0
22	MG	A	3558	1/1	0.93	0.19	108,108,108,108	0
22	MG	A	3433	1/1	0.93	0.12	87,87,87,87	0
22	MG	A	3593	1/1	0.93	0.16	110,110,110,110	0
22	MG	A	3519	1/1	0.93	0.09	103,103,103,103	0
22	MG	A	3522	1/1	0.93	0.24	73,73,73,73	0
22	MG	A	3497	1/1	0.93	0.20	82,82,82,82	0
22	MG	A	3546	1/1	0.93	0.14	110,110,110,110	0
23	ZN	D	301	1/1	0.93	0.37	121,121,121,121	0
22	MG	A	3463	1/1	0.93	0.11	80,80,80,80	0
22	MG	A	3559	1/1	0.94	0.20	104,104,104,104	0
22	MG	A	3441	1/1	0.94	0.33	76,76,76,76	0

Continued on next page...

Continued from previous page...

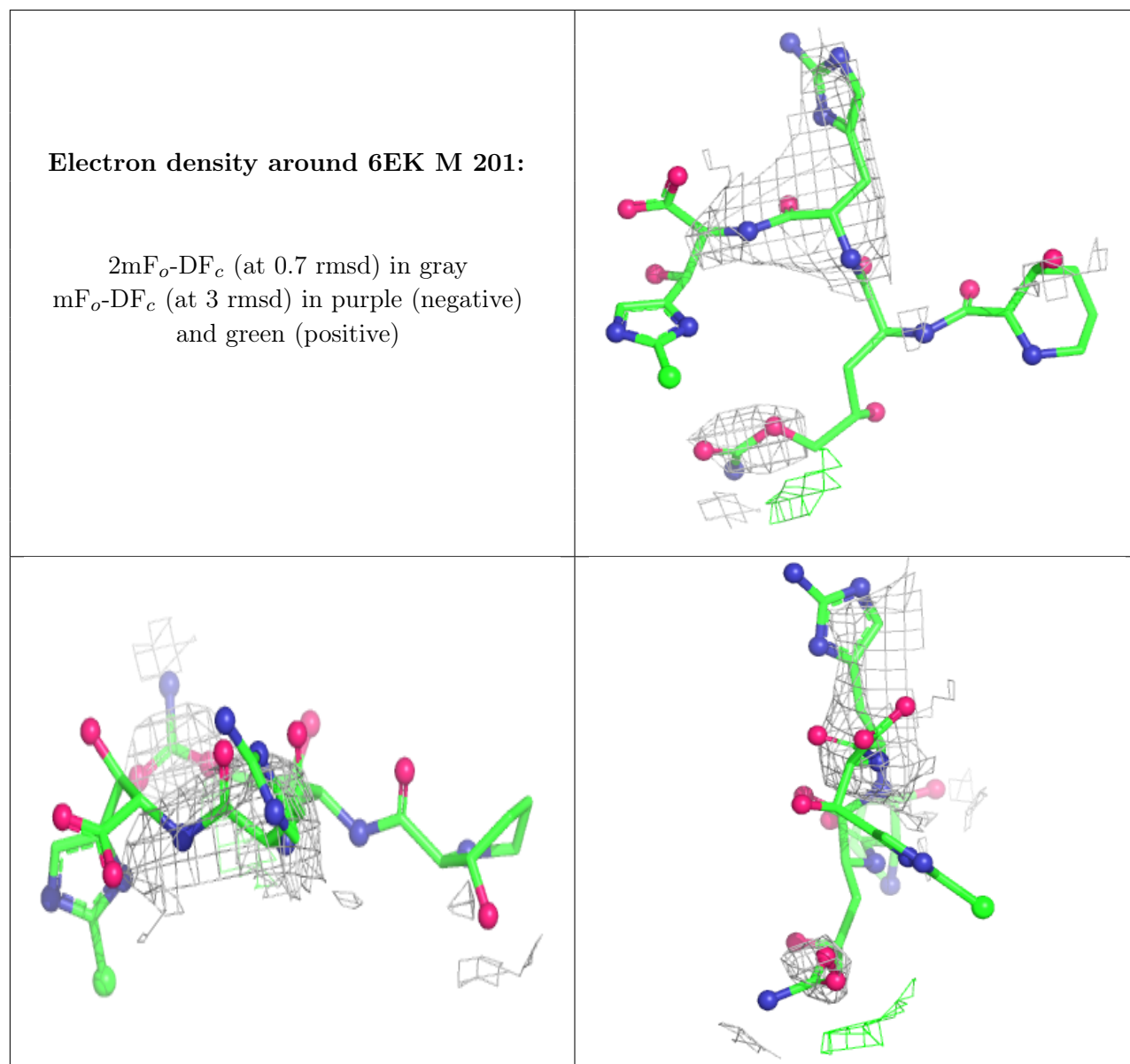
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	MG	A	3402	1/1	0.94	0.21	93,93,93,93	0
22	MG	A	3549	1/1	0.94	0.19	116,116,116,116	0
22	MG	A	3445	1/1	0.94	0.13	75,75,75,75	0
22	MG	A	3446	1/1	0.94	0.24	68,68,68,68	0
22	MG	A	3413	1/1	0.94	0.18	94,94,94,94	0
22	MG	A	3454	1/1	0.94	0.15	87,87,87,87	0
22	MG	A	3455	1/1	0.94	0.25	67,67,67,67	0
22	MG	A	3490	1/1	0.94	0.19	118,118,118,118	0
22	MG	A	3521	1/1	0.94	0.32	73,73,73,73	0
22	MG	A	3548	1/1	0.95	0.06	97,97,97,97	0
22	MG	A	3423	1/1	0.95	0.24	75,75,75,75	0
22	MG	A	3568	1/1	0.95	0.16	76,76,76,76	0
22	MG	A	3458	1/1	0.95	0.21	65,65,65,65	0
22	MG	A	3459	1/1	0.95	0.12	83,83,83,83	0
22	MG	A	3475	1/1	0.95	0.21	94,94,94,94	0
22	MG	A	3572	1/1	0.95	0.21	118,118,118,118	0
22	MG	A	3487	1/1	0.95	0.19	84,84,84,84	0
22	MG	A	3591	1/1	0.95	0.06	116,116,116,116	0
22	MG	A	3421	1/1	0.95	0.11	83,83,83,83	0
22	MG	A	3447	1/1	0.95	0.18	72,72,72,72	0
22	MG	A	3437	1/1	0.95	0.22	66,66,66,66	0
22	MG	A	3542	1/1	0.95	0.11	139,139,139,139	0
22	MG	A	3503	1/1	0.95	0.16	101,101,101,101	0
22	MG	H	201	1/1	0.95	0.18	69,69,69,69	0
22	MG	A	3580	1/1	0.95	0.17	91,91,91,91	0
22	MG	A	3444	1/1	0.95	0.11	75,75,75,75	0
22	MG	A	3436	1/1	0.96	0.09	94,94,94,94	0
22	MG	K	201	1/1	0.96	0.21	83,83,83,83	0
22	MG	A	3478	1/1	0.96	0.12	76,76,76,76	0
22	MG	A	3536	1/1	0.96	0.17	93,93,93,93	0
22	MG	A	3537	1/1	0.96	0.13	81,81,81,81	0
22	MG	A	3428	1/1	0.96	0.12	98,98,98,98	0
22	MG	A	3480	1/1	0.96	0.31	68,68,68,68	0
22	MG	A	3460	1/1	0.96	0.42	74,74,74,74	0
22	MG	A	3470	1/1	0.96	0.07	106,106,106,106	0
22	MG	A	3461	1/1	0.96	0.10	89,89,89,89	0
22	MG	E	201	1/1	0.96	0.30	67,67,67,67	0
22	MG	A	3419	1/1	0.96	0.20	81,81,81,81	0
22	MG	A	3596	1/1	0.96	0.25	108,108,108,108	0
22	MG	A	3545	1/1	0.96	0.07	118,118,118,118	0
22	MG	A	3520	1/1	0.96	0.25	71,71,71,71	0
22	MG	A	3565	1/1	0.96	0.16	81,81,81,81	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	MG	A	3566	1/1	0.96	0.27	88,88,88,88	0
22	MG	A	3496	1/1	0.97	0.14	98,98,98,98	0
22	MG	A	3553	1/1	0.97	0.11	77,77,77,77	0
22	MG	A	3560	1/1	0.97	0.13	71,71,71,71	0
22	MG	A	3471	1/1	0.97	0.15	70,70,70,70	0
22	MG	A	3525	1/1	0.97	0.13	79,79,79,79	0
22	MG	A	3443	1/1	0.97	0.21	72,72,72,72	0
22	MG	A	3498	1/1	0.98	0.08	78,78,78,78	0
22	MG	A	3584	1/1	0.98	0.10	97,97,97,97	0
22	MG	A	3462	1/1	0.98	0.08	73,73,73,73	0
22	MG	A	3504	1/1	0.98	0.07	98,98,98,98	0
22	MG	A	3547	1/1	0.98	0.04	94,94,94,94	0
22	MG	A	3555	1/1	0.98	0.09	110,110,110,110	0
22	MG	A	3505	1/1	0.98	0.11	122,122,122,122	0
22	MG	A	3420	1/1	0.98	0.15	78,78,78,78	0
22	MG	A	3466	1/1	0.98	0.11	74,74,74,74	0
22	MG	A	3472	1/1	0.99	0.04	94,94,94,94	0
22	MG	A	3434	1/1	0.99	0.07	77,77,77,77	0
22	MG	A	3415	1/1	0.99	0.10	64,64,64,64	0
23	ZN	N	101	1/1	1.00	0.01	144,144,144,144	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.