



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 10:22 PM GMT

PDB ID : 5C8Y
Title : Crystal structure of T2R-TTL-Plinabulin complex
Authors : Wang, Y.; Yu, Y.; Chen, Q.; Yang, J.
Deposited on : 2015-06-26
Resolution : 2.59 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20026982

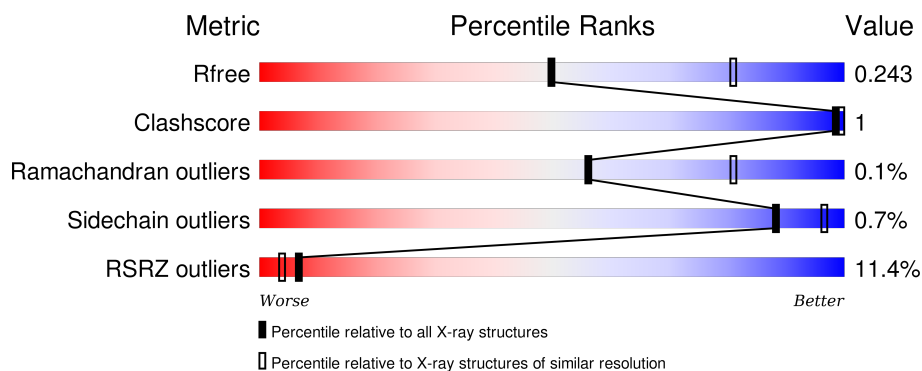
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	450	<div> <div>6%</div> <div>96%</div> <div>..</div> </div>
1	C	450	<div> <div>2%</div> <div>96%</div> <div>..</div> </div>
2	B	445	<div> <div>7%</div> <div>92%</div> <div>. .</div> </div>
2	D	445	<div> <div>13%</div> <div>92%</div> <div>. 5%</div> </div>
3	E	143	<div> <div>10%</div> <div>84%</div> <div>. 15%</div> </div>

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Mol	Chain	Length	Quality of chain
4	F	384	<p>28% 83% 13%</p>

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
6	MG	C	502	-	-	-	X

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 34616 atoms, of which 16867 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 Tubulin alpha.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	437	Total	C	H	N	O	S	0	0	0
			6733	2163	3317	581	650	22			
1	C	440	Total	C	H	N	O	S	0	0	0
			6772	2175	3335	584	656	22			

- Molecule 2 is a protein called Tubulin beta.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	427	Total	C	H	N	O	S	0	0	0
			6589	2110	3228	576	649	26			
2	D	421	Total	C	H	N	O	S	0	0	0
			6488	2080	3179	562	640	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	121	Total	C	H	N	O	S	0	0	0
			2014	617	1014	181	197	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	expression tag	UNP P63043
E	4	ALA	-	expression tag	UNP P63043

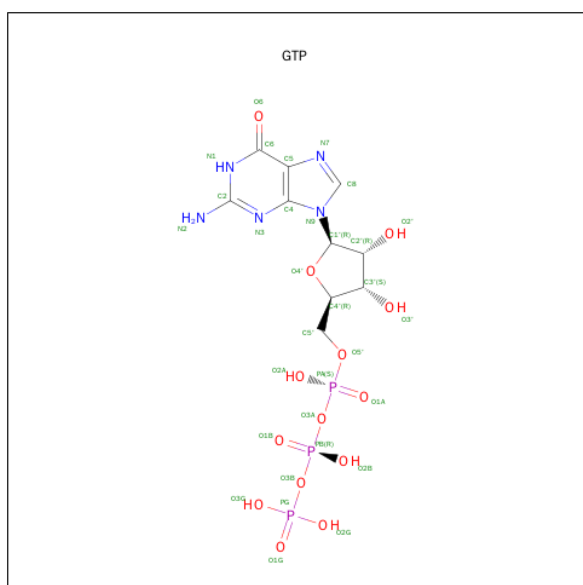
- Molecule 4 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	F	334	Total	C	H	N	O	S	0	0	0
			5442	1761	2698	470	499	14			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP E1BQ43
F	380	HIS	-	expression tag	UNP E1BQ43
F	381	HIS	-	expression tag	UNP E1BQ43
F	382	HIS	-	expression tag	UNP E1BQ43
F	383	HIS	-	expression tag	UNP E1BQ43
F	384	HIS	-	expression tag	UNP E1BQ43

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	P	0	0
			42	10	10	5	14	3		
5	C	1	Total	C	H	N	O	P	0	0
			42	10	10	5	14	3		

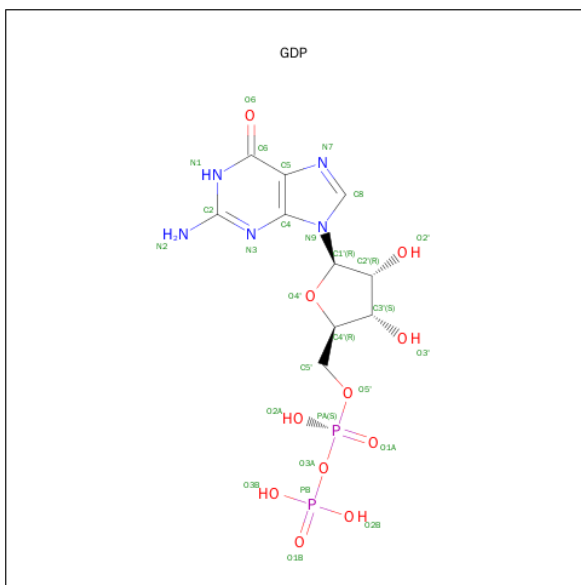
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Mg	0	0
			1	1		
6	A	1	Total	Mg	0	0
			1	1		
6	C	1	Total	Mg	0	0
			1	1		

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Ca 1 1	0	0
7	C	1	Total Ca 1 1	0	0

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



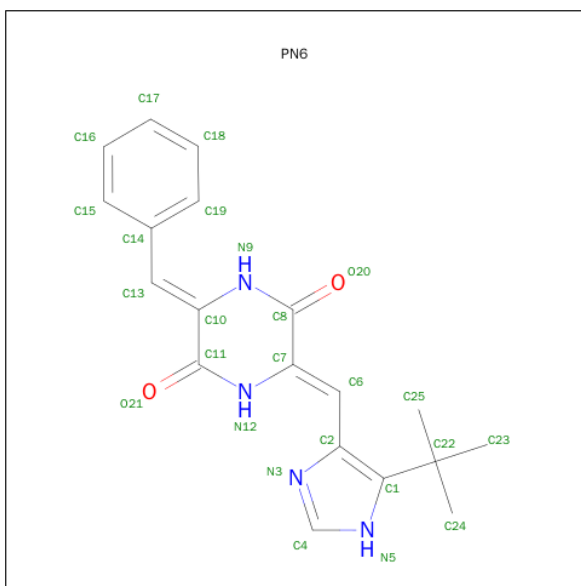
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	B	1	Total	C	H	N	O	P	0	0
			38	10	10	5	11	2		
8	D	1	Total	C	H	N	O	P	0	0
			38	10	10	5	11	2		

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



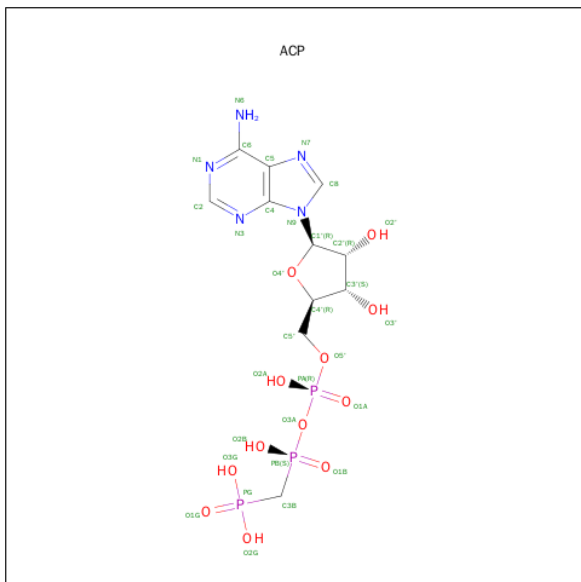
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	H	N	O	S	
			24	6	12	1	4	1	

- Molecule 10 is (3Z,6Z)-3-benzylidene-6-[(5-tert-butyl-1H-imidazol-4-yl)methylidene]piperazine-2,5-dione (three-letter code: PN6) (formula: C₁₉H₂₀N₄O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	H	N	O		
			45	19	20	4	2	0	0
10	D	1	Total	C	H	N	O		
			45	19	20	4	2	0	0

- Molecule 11 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	F	1	Total	C	H	N	O	P	
			35	11	4	5	12	3	
								0	0

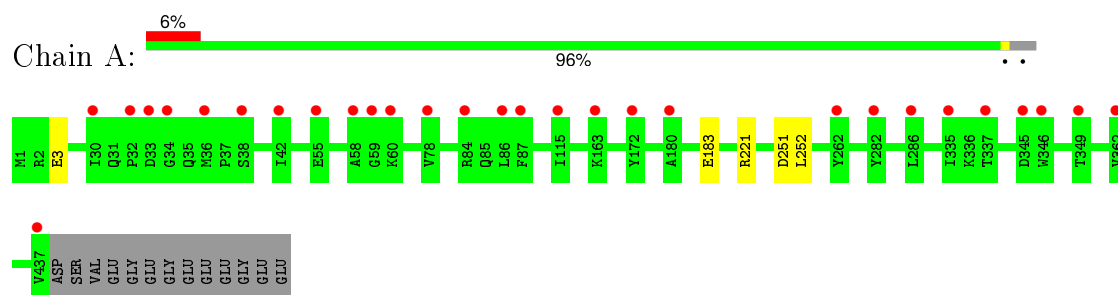
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	68	Total	O		
			68	68	0	0
12	B	49	Total	O		
			49	49	0	0
12	C	89	Total	O		
			89	89	0	0
12	D	20	Total	O		
			20	20	0	0
12	E	13	Total	O		
			13	13	0	0
12	F	25	Total	O		
			25	25	0	0

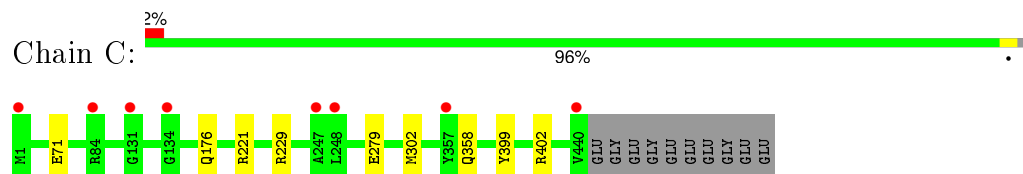
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

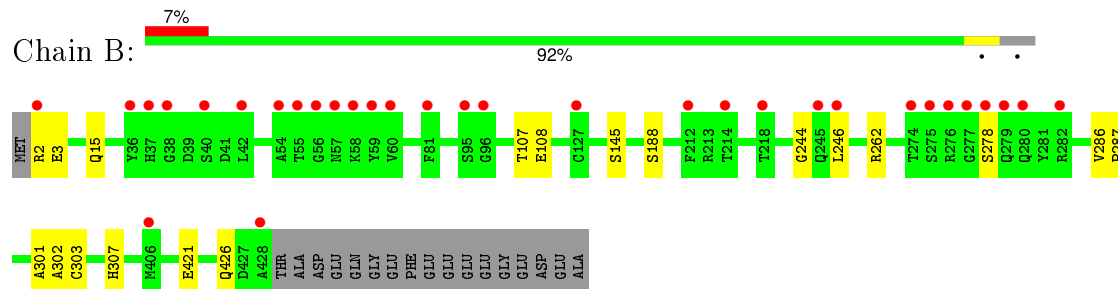
• Molecule 1: Tubulin alpha



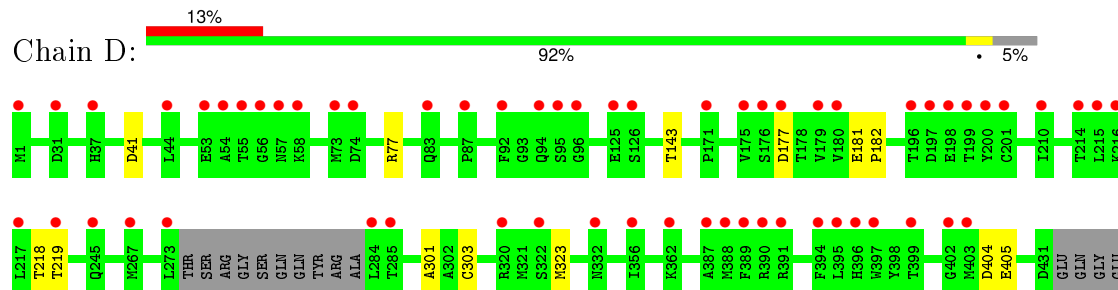
• Molecule 1: Tubulin alpha



• Molecule 2: Tubulin beta

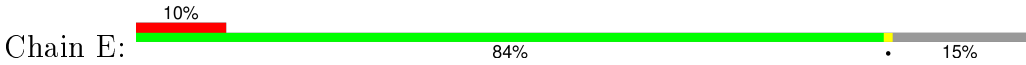


• Molecule 2: Tubulin beta



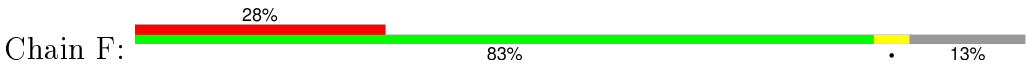
PHE
GLU
GLU
GLU
GLY
GLU
ASP
GLU
ALA

● Molecule 3: Stathmin-4



RET
ALA
ASP
P6
E7
V8
I9
I23
I24
I25
P26
P27
S28
PHE
ASP
GLY
VAL
PRO
GLU
PHE
ASN
ALA
SER
LEU
PRO
ARG
ARG
ARG
D44
P45
S46
Q103
E106
L120
K135
L139
K140
E141
GLU
ALA
SER
ARG

● Molecule 4: Uncharacterized protein



H1
E3
V17
R18
R19
L20
L21
L22
A23
T24
G25
Q26
K27
K28
R31
K74
S88
T92
Y98
Y99
I100
Y101
P102
T103
ASN
LEU
LYS
THR
PRO
VAL
ALA
PRO
ALA
GLN
ASN
GLY
ILE
ANG
HIS
LEU
ILE
ASN
ASN
THR
ARG
THR
D126
E127
R128
E129
V130
F131
L132
A133
A134
Y135
N136
R137
R138
R139
R142
E143
G144
N145
V146
W147
I148
A149
LYS
SER
SER
ALA
ALA
LYS
GLY
GLY
ILE
L161
I162
S163
S164
E165
A166
S167
E168
L169
L170
D171
F172
I173
D174
E175
G176
G177
Q178
V179
H180
V181
I182
Q183
K184
Y185
L191
L192
E193
F194
K198
F199
D208
N212
L221
R222
T223
S224
E225
E226
P227
S230
A231
N232
F233
Q234
D235
K236
L240
T241
N242
H243
C244
I245
Q246
K247
GLU
TYR
SER
LYS
N252
Y253
G254
R255
Y256
E257
E258
G259
N260
E261
M262
F263
M296
E299
P300
K305
Q310
G316
F317
D318
M320
E331
C338
A339
Q340
Y341
L342
V351
L361
A362
ASP
THR
GLY
GLN
LYS
THR
SER
GLN
PRO
T372
S373
L374
H379
H380
HIS
HIS
HIS

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.06Å 158.44Å 181.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.70 – 2.59 45.48 – 2.59	Depositor EDS
% Data completeness (in resolution range)	98.8 (39.70-2.59) 98.8 (45.48-2.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 2.58Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.222 , 0.271 0.237 , 0.243	Depositor DCC
R_{free} test set	4634 reflections (5.22%)	DCC
Wilson B-factor (Å ²)	44.9	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 59.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 93387 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	34616	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GDP, MG, CA, PN6, GTP, ACP, MES

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	0.22	0/3494	0.37	0/4743
1	C	0.22	0/3515	0.37	0/4772
2	B	0.22	0/3436	0.38	0/4654
2	D	0.22	0/3382	0.37	0/4581
3	E	0.21	0/1008	0.32	0/1337
4	F	0.22	0/2806	0.36	0/3791
All	All	0.22	0/17641	0.37	0/23878

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3416	3317	3330	3	0
1	C	3437	3335	3348	5	0
2	B	3361	3228	3238	8	0
2	D	3309	3179	3189	6	0
3	E	1000	1014	1018	1	0
4	F	2744	2698	2709	7	0
5	A	32	10	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	10	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	B	28	10	12	0	0
8	D	28	10	12	1	0
9	B	12	12	12	0	0
10	B	25	20	20	0	0
10	D	25	20	20	1	0
11	F	31	4	14	0	0
12	A	68	0	0	0	0
12	B	49	0	0	1	0
12	C	89	0	0	3	0
12	D	20	0	0	1	0
12	E	13	0	0	1	0
12	F	25	0	0	0	0
All	All	17749	16867	16946	31	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 1.

All (31) 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)
2:B:2:ARG:NH1	12:B:603:HOH:O	2.27	0.67
2:D:77:ARG:NH2	12:D:1201:HOH:O	2.30	0.64
4:F:222:ARG:NH1	4:F:318:ASP:OD1	2.33	0.62
2:B:301:ALA:O	2:B:303:CYS:N	2.32	0.61
2:D:404:ASP:OD1	2:D:405:GLU:N	2.35	0.59
1:C:176:GLN:NE2	12:C:604:HOH:O	2.35	0.58
1:A:251:ASP:OD1	1:A:252:LEU:N	2.37	0.58
4:F:185:TYR:OH	4:F:198:LYS:NZ	2.39	0.56
1:C:229:ARG:NH2	12:C:606:HOH:O	2.38	0.56
2:B:145:SER:HG	2:B:188:SER:HG	1.53	0.56
2:D:143:THR:N	8:D:501:GDP:O2B	2.43	0.51
10:D:502:PN6:N12	10:D:502:PN6:N3	2.49	0.51
2:B:262:ARG:NE	2:B:421:GLU:OE2	2.45	0.49
4:F:178:GLN:OE1	4:F:178:GLN:N	2.45	0.49
1:C:399:TYR:O	1:C:402:ARG:NH2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:279:GLU:OE1	1:C:279:GLU:N	2.46	0.46
1:C:71:GLU:O	12:C:601:HOH:O	2.20	0.46
2:D:301:ALA:O	2:D:303:CYS:N	2.48	0.45
2:D:181:GLU:N	2:D:182:PRO:HD2	2.31	0.45
4:F:208:ASP:OD1	4:F:212:ASN:N	2.47	0.44
2:B:307:HIS:O	2:B:426:GLN:NE2	2.51	0.43
1:A:183:GLU:OE2	5:A:501:GTP:O3'	2.20	0.43
3:E:6:MET:N	12:E:204:HOH:O	2.51	0.43
4:F:338:CYS:SG	4:F:339:ALA:N	2.92	0.42
4:F:184:LYS:NZ	4:F:185:TYR:O	2.51	0.42
2:B:107:THR:OG1	2:B:108:GLU:N	2.53	0.41
2:B:3:GLU:OE2	2:B:3:GLU:N	2.53	0.41
2:D:218:THR:O	2:D:219:THR:OG1	2.37	0.41
1:A:3:GLU:N	1:A:3:GLU:OE1	2.54	0.40
2:B:286:VAL:HB	2:B:287:PRO:HD3	2.03	0.40
4:F:299:GLU:N	4:F:300:PRO:HD2	2.36	0.40

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	A	435/450 (97%)	414 (95%)	21 (5%)	0	100	100
1	C	438/450 (97%)	427 (98%)	11 (2%)	0	100	100
2	B	425/445 (96%)	408 (96%)	14 (3%)	3 (1%)	26	51
2	D	417/445 (94%)	401 (96%)	16 (4%)	0	100	100
3	E	117/143 (82%)	115 (98%)	2 (2%)	0	100	100
4	F	324/384 (84%)	312 (96%)	12 (4%)	0	100	100
All	All	2156/2317 (93%)	2077 (96%)	76 (4%)	3 (0%)	56	81

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	244	GLY
2	B	302	ALA
2	B	278	SER

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	368/378 (97%)	367 (100%)	1 (0%)	94	99
1	C	371/378 (98%)	368 (99%)	3 (1%)	86	95
2	B	369/383 (96%)	367 (100%)	2 (0%)	92	98
2	D	364/383 (95%)	361 (99%)	3 (1%)	86	95
3	E	109/127 (86%)	109 (100%)	0	100	100
4	F	301/342 (88%)	296 (98%)	5 (2%)	68	88
All	All	1882/1991 (94%)	1868 (99%)	14 (1%)	88	96

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	221	ARG
2	B	15	GLN
2	B	246	LEU
1	C	221	ARG
1	C	302	MET
1	C	358	GLN
2	D	41	ASP
2	D	177	ASP
2	D	323	MET
4	F	88	SER
4	F	92	THR
4	F	296	MET
4	F	310	GLN
4	F	331	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 5 are monoatomic - leaving 8 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	$\# Z > 2$
5	GTP	A	501	6	26,34,34	1.08	1 (3%)	26,54,54	0.85	0
8	GDP	B	501	6	24,30,30	1.39	4 (16%)	23,47,47	0.87	0
9	MES	B	503	-	12,12,12	1.93	1 (8%)	15,16,16	1.84	3 (20%)
10	PN6	B	504	-	20,27,27	1.70	6 (30%)	19,39,39	1.62	1 (5%)
5	GTP	C	501	6	26,34,34	1.08	1 (3%)	26,54,54	0.89	0
8	GDP	D	501	-	24,30,30	1.40	4 (16%)	23,47,47	0.88	0
10	PN6	D	502	-	20,27,27	1.80	5 (25%)	19,39,39	1.42	1 (5%)
11	ACP	F	401	-	29,33,33	1.83	7 (24%)	29,52,52	1.79	3 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means

no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GTP	A	501	6	-	0/18/38/38	0/3/3/3
8	GDP	B	501	6	-	0/12/32/32	0/3/3/3
9	MES	B	503	-	-	0/6/14/14	0/1/1/1
10	PN6	B	504	-	-	0/10/14/14	0/3/3/3
5	GTP	C	501	6	-	0/18/38/38	0/3/3/3
8	GDP	D	501	-	-	0/12/32/32	0/3/3/3
10	PN6	D	502	-	-	0/10/14/14	0/3/3/3
11	ACP	F	401	-	-	0/15/38/38	0/3/3/3

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	503	MES	C8-S	-6.29	1.66	1.78
11	F	401	ACP	PB-O2B	-3.92	1.46	1.56
10	B	504	PN6	C14-C13	-3.48	1.39	1.46
10	D	502	PN6	C14-C13	-3.45	1.39	1.46
11	F	401	ACP	PG-O2G	-3.27	1.46	1.54
11	F	401	ACP	C2'-C1'	-2.85	1.49	1.53
8	B	501	GDP	C2-N3	2.07	1.36	1.33
11	F	401	ACP	C5-C4	2.12	1.45	1.40
10	D	502	PN6	C11-N12	2.13	1.39	1.36
10	B	504	PN6	C11-N12	2.22	1.39	1.36
10	B	504	PN6	C7-N12	2.22	1.40	1.36
11	F	401	ACP	PG-O3G	2.23	1.60	1.54
8	D	501	GDP	C2-N3	2.25	1.36	1.33
8	B	501	GDP	C2-N2	2.49	1.36	1.32
8	D	501	GDP	C2-N2	2.51	1.36	1.32
10	B	504	PN6	C10-N9	2.57	1.40	1.36
8	B	501	GDP	C5-C4	2.92	1.47	1.40
8	D	501	GDP	C5-C4	2.97	1.47	1.40
10	D	502	PN6	C22-C1	3.05	1.57	1.52
10	B	504	PN6	C22-C1	3.12	1.57	1.52
10	D	502	PN6	C10-N9	3.14	1.41	1.36
11	F	401	ACP	PB-O1B	3.31	1.60	1.51
10	B	504	PN6	C8-N9	3.42	1.41	1.36
8	D	501	GDP	C6-C5	3.88	1.48	1.40
8	B	501	GDP	C6-C5	3.90	1.48	1.40
5	C	501	GTP	C2-N3	4.08	1.38	1.33
5	A	501	GTP	C2-N3	4.08	1.38	1.33
10	D	502	PN6	C8-N9	4.09	1.42	1.36
11	F	401	ACP	PG-O1G	5.06	1.61	1.50

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	F	401	ACP	N3-C2-N1	-6.79	123.54	128.87
10	B	504	PN6	C10-C13-C14	-6.10	122.05	130.26
10	D	502	PN6	C10-C13-C14	-5.28	123.16	130.26
11	F	401	ACP	O2'-C2'-C1'	-2.44	103.99	111.61
11	F	401	ACP	O2'-C2'-C3'	-2.40	104.09	111.86
9	B	503	MES	C7-N4-C3	2.21	116.05	111.25
9	B	503	MES	C7-N4-C5	3.07	117.94	111.25
9	B	503	MES	C5-N4-C3	4.69	119.38	108.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	501	GTP	1	0
8	D	501	GDP	1	0
10	D	502	PN6	1	0

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	437/450 (97%)	0.79	29 (6%)	22 16	27, 49, 78, 145	0
1	C	440/450 (97%)	0.26	8 (1%)	71 66	21, 37, 66, 90	0
2	B	427/445 (95%)	0.65	32 (7%)	17 12	23, 47, 88, 121	0
2	D	421/445 (94%)	1.01	60 (14%)	4 2	33, 65, 102, 124	0
3	E	121/143 (84%)	1.04	14 (11%)	6 4	30, 67, 100, 127	0
4	F	334/384 (86%)	1.62	106 (31%)	1 0	38, 76, 126, 153	0
All	All	2180/2317 (94%)	0.84	249 (11%)	7 4	21, 54, 102, 153	0

All (249) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	282	TYR	8.6
4	F	233	PHE	8.1
4	F	234	GLN	8.0
4	F	161	LEU	7.6
4	F	169	LEU	7.2
2	D	394	PHE	7.2
4	F	132	LEU	7.0
4	F	173	ILE	6.5
2	D	1	MET	6.4
2	D	55	THR	6.4
4	F	142	ARG	6.2
4	F	103	THR	5.8
4	F	100	ILE	5.8
4	F	167	SER	5.8
4	F	245	ILE	5.7
4	F	135	TYR	5.7
4	F	232	ASN	5.6
4	F	253	TYR	5.6
4	F	170	LEU	5.3

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Mol	Chain	Res	Type	RSRZ
2	D	94	GLN	5.0
4	F	225	SER	4.9
4	F	172	PHE	4.9
2	D	390	ARG	4.9
4	F	178	GLN	4.9
2	B	279	GLN	4.9
4	F	372	THR	4.8
4	F	194	PRO	4.8
4	F	162	ILE	4.7
4	F	256	TYR	4.5
4	F	180	HIS	4.5
2	D	92	PHE	4.5
2	D	397	TRP	4.4
4	F	168	GLU	4.4
4	F	31	ARG	4.4
4	F	130	VAL	4.3
4	F	182	ILE	4.2
4	F	240	LEU	4.2
2	D	216	LYS	4.2
2	D	37	HIS	4.2
4	F	139	ARG	4.2
4	F	227	PRO	4.2
4	F	101	TYR	4.2
2	B	280	GLN	4.2
4	F	361	LEU	4.1
2	D	391	ARG	4.1
2	B	37	HIS	4.1
2	B	245	GLN	4.0
2	D	54	ALA	4.0
2	D	389	PHE	4.0
2	D	180	VAL	4.0
4	F	98	TYR	3.9
4	F	255	ARG	3.9
1	A	86	LEU	3.9
3	E	139	LEU	3.9
2	D	356	ILE	3.7
4	F	252	ASN	3.7
2	D	396	HIS	3.7
4	F	246	GLN	3.7
2	D	56	GLY	3.7
4	F	25	GLY	3.7
3	E	27	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
2	B	282	ARG	3.6
2	D	177	ASP	3.6
3	E	24	LEU	3.6
4	F	27	TRP	3.5
4	F	243	HIS	3.5
2	D	285	THR	3.5
4	F	231	ALA	3.5
4	F	235	ASP	3.5
4	F	128	ARG	3.5
4	F	137	ARG	3.5
4	F	223	THR	3.5
4	F	236	LYS	3.5
4	F	176	GLN	3.4
4	F	133	ALA	3.4
4	F	199	PHE	3.4
2	D	53	GLU	3.4
4	F	175	GLU	3.4
4	F	254	GLY	3.4
1	A	34	GLY	3.4
2	B	55	THR	3.4
2	D	245	GLN	3.3
2	B	95	SER	3.3
4	F	136	ASN	3.3
2	B	276	ARG	3.3
2	D	219	THR	3.3
2	B	277	GLY	3.3
4	F	258	GLU	3.3
3	E	6	MET	3.3
2	D	214	THR	3.2
4	F	171	ASP	3.2
2	D	322	SER	3.2
2	D	96	GLY	3.2
2	D	87	PRO	3.2
4	F	145	ASN	3.2
1	C	247	ALA	3.2
2	D	217	LEU	3.2
2	D	362	LYS	3.1
4	F	179	VAL	3.1
2	D	320	ARG	3.1
2	D	74	ASP	3.1
4	F	129	GLU	3.1
3	E	135	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
2	D	200	TYR	3.1
1	A	437	VAL	3.1
4	F	380	HIS	3.1
2	B	278	SER	3.0
1	C	440	VAL	3.0
1	A	42	ILE	3.0
4	F	165	GLU	3.0
4	F	247	LYS	3.0
2	D	395	LEU	3.0
3	E	7	GLU	3.0
2	D	215	LEU	3.0
4	F	163	SER	2.9
4	F	17	VAL	2.9
4	F	20	LEU	2.9
4	F	22	LEU	2.9
2	D	388	MET	2.9
1	A	59	GLY	2.9
1	A	163	LYS	2.9
4	F	138	ARG	2.9
2	B	96	GLY	2.8
2	D	73	MET	2.8
2	D	176	SER	2.8
1	A	180	ALA	2.8
2	B	218	THR	2.8
1	C	357	TYR	2.8
2	D	95	SER	2.8
2	B	127	CYS	2.8
4	F	362	ALA	2.8
4	F	191	LEU	2.8
4	F	1	MET	2.8
4	F	147	TRP	2.8
4	F	226	GLU	2.7
4	F	149	ALA	2.7
4	F	305	LYS	2.7
2	B	56	GLY	2.7
1	A	345	ASP	2.7
4	F	19	ARG	2.7
3	E	106	GLU	2.7
4	F	21	LEU	2.7
4	F	379	HIS	2.7
2	D	171	PRO	2.7
2	D	175	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	54	ALA	2.7
3	E	46	SER	2.7
2	B	275	SER	2.7
2	B	81	PHE	2.7
3	E	9	ILE	2.7
4	F	146	VAL	2.6
4	F	24	THR	2.6
2	D	126	SER	2.6
2	D	179	VAL	2.6
1	A	262	TYR	2.6
2	B	246	LEU	2.6
1	A	60	LYS	2.6
2	D	58	LYS	2.6
4	F	260	ASN	2.6
2	B	38	GLY	2.6
4	F	102	PRO	2.6
4	F	131	PHE	2.6
3	E	103	GLN	2.6
2	B	57	ASN	2.6
2	D	197	ASP	2.6
2	B	2	ARG	2.5
4	F	177	GLY	2.5
4	F	143	GLU	2.5
2	D	387	ALA	2.5
3	E	25	LYS	2.5
2	D	57	ASN	2.5
2	D	199	THR	2.5
4	F	23	ALA	2.5
1	C	248	LEU	2.5
4	F	166	ALA	2.5
2	B	406	MET	2.5
1	A	335	ILE	2.5
2	D	201	CYS	2.5
1	A	78	VAL	2.5
3	E	23	ILE	2.5
4	F	320	MET	2.5
4	F	221	LEU	2.4
4	F	340	GLN	2.4
4	F	185	TYR	2.4
4	F	316	GLY	2.4
1	A	349	THR	2.4
2	B	428	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
4	F	192	LEU	2.4
2	B	58	LYS	2.4
4	F	74	LYS	2.4
1	C	1	MET	2.4
2	D	267	MET	2.4
4	F	164	SER	2.4
4	F	263	PHE	2.4
4	F	241	THR	2.4
2	D	198	GLU	2.4
2	B	59	TYR	2.3
1	A	38	SER	2.3
2	D	284	LEU	2.3
1	A	362	VAL	2.3
2	B	212	PHE	2.3
2	D	332	ASN	2.3
2	D	125	GLU	2.3
2	B	36	TYR	2.3
4	F	174	ASP	2.3
2	D	210	ILE	2.3
2	D	399	THR	2.3
1	C	84	ARG	2.3
1	A	115	ILE	2.3
3	E	140	LYS	2.2
4	F	28	LYS	2.2
2	B	42	LEU	2.2
2	D	196	THR	2.2
1	C	134	GLY	2.2
2	B	40	SER	2.2
4	F	127	GLU	2.2
4	F	351	VAL	2.2
4	F	259	GLY	2.2
1	A	32	PRO	2.2
4	F	257	GLU	2.2
1	A	30	ILE	2.1
1	C	131	GLY	2.1
4	F	374	ILE	2.1
2	D	83	GLN	2.1
2	D	31	ASP	2.1
1	A	55	GLU	2.1
4	F	262	MET	2.1
2	D	402	GLY	2.1
1	A	36	MET	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	403	MET	2.1
1	A	172	TYR	2.1
1	A	84	ARG	2.1
2	D	44	LEU	2.1
4	F	9	GLU	2.1
1	A	87	PHE	2.1
1	A	286	LEU	2.1
2	D	273	LEU	2.1
1	A	346	TRP	2.1
1	A	337	THR	2.0
4	F	224	SER	2.0
4	F	342	LEU	2.0
1	A	33	ASP	2.0
1	A	58	ALA	2.0
2	B	60	VAL	2.0
4	F	99	VAL	2.0
3	E	120	LEU	2.0
2	B	214	THR	2.0
2	B	274	THR	2.0
4	F	230	SER	2.0

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
6	MG	C	502	1/1	0.96	0.33	5.32	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
10	PN6	D	502	25/25	0.87	0.32	1.77	41,77,120,145	0
8	GDP	B	501	28/28	0.94	0.23	1.62	18,38,62,71	0
10	PN6	B	504	25/25	0.95	0.25	0.94	30,51,79,97	0
5	GTP	C	501	32/32	0.97	0.21	0.73	16,32,53,91	0
5	GTP	A	501	32/32	0.96	0.24	0.33	13,35,46,79	0
6	MG	A	502	1/1	0.95	0.23	0.27	26,26,26,26	0
9	MES	B	503	12/12	0.91	0.19	-0.01	38,57,82,89	0
8	GDP	D	501	28/28	0.90	0.19	-0.51	35,64,100,112	0
11	ACP	F	401	31/31	0.88	0.20	-1.28	72,107,155,168	0
7	CA	C	503	1/1	0.98	0.11	-1.48	55,55,55,55	0
7	CA	A	503	1/1	0.82	0.10	-1.75	76,76,76,76	0
6	MG	B	502	1/1	0.95	0.32	-	40,40,40,40	0

6.5 Other polymers ⓘ

There are no such residues in this entry.