Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 10:14 PM BST

PDB ID	:	6Y3Z
Title	:	Crystal structure of the Pby1 ATP-grasp enzyme bound to the S. cerevisiae mRNA decapping complex (Dcp1-Dcp2-Edc3)
Authors	:	Graille, M.
Deposited on	:	2020-02-19
Resolution	:	3.49 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

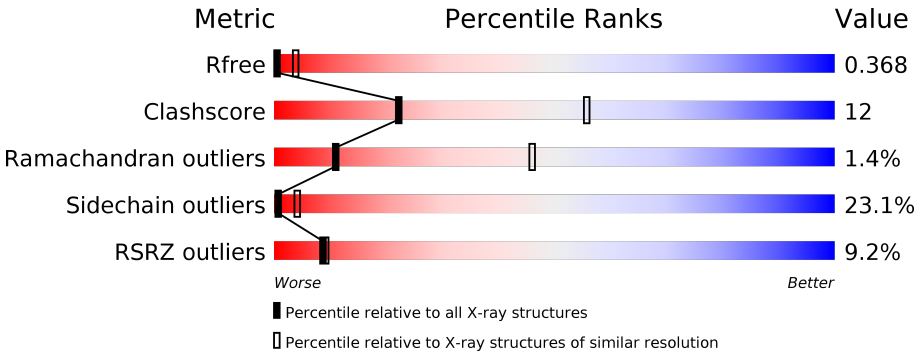
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.49 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	277	13% 52% 31% 5% 12%
2	B	236	5% 92%
3	C	71	8% 56% 21% 11% 11%
4	P	429	5% 42% 31% 7% 19%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5570 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 m7GpppN-mRNA hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	243	Total	C	N	O	S	0	0	0
			2044	1323	338	374	9			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	272	HIS	-	expression tag	UNP P53550
A	273	HIS	-	expression tag	UNP P53550
A	274	HIS	-	expression tag	UNP P53550
A	275	HIS	-	expression tag	UNP P53550
A	276	HIS	-	expression tag	UNP P53550
A	277	HIS	-	expression tag	UNP P53550

- Molecule 2 is a protein called mRNA-decapping enzyme subunit 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	18	Total	C	N	O	0	0	0
			159	104	28	27			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	GLY	-	expression tag	UNP Q12517
B	-3	PRO	-	expression tag	UNP Q12517
B	-2	LEU	-	expression tag	UNP Q12517
B	-1	GLY	-	expression tag	UNP Q12517
B	0	SER	-	expression tag	UNP Q12517

- Molecule 3 is a protein called Enhancer of mRNA-decapping protein 3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	63	Total	C	N	O	0	0	0
			470	299	84	87			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	GLY	-	expression tag	UNP P39998
C	-3	PRO	-	expression tag	UNP P39998
C	-2	LEU	-	expression tag	UNP P39998
C	-1	GLY	-	expression tag	UNP P39998
C	0	SER	-	expression tag	UNP P39998

- Molecule 4 is a protein called Probable tubulin–tyrosine ligase PBY1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	P	348	Total	C	N	O	S	0	0	0
			2896	1868	461	558	9			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	325	GLY	-	expression tag	UNP P38254
P	326	PRO	-	expression tag	UNP P38254
P	327	LEU	-	expression tag	UNP P38254
P	328	GLY	-	expression tag	UNP P38254
P	329	SER	-	expression tag	UNP P38254

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by author).

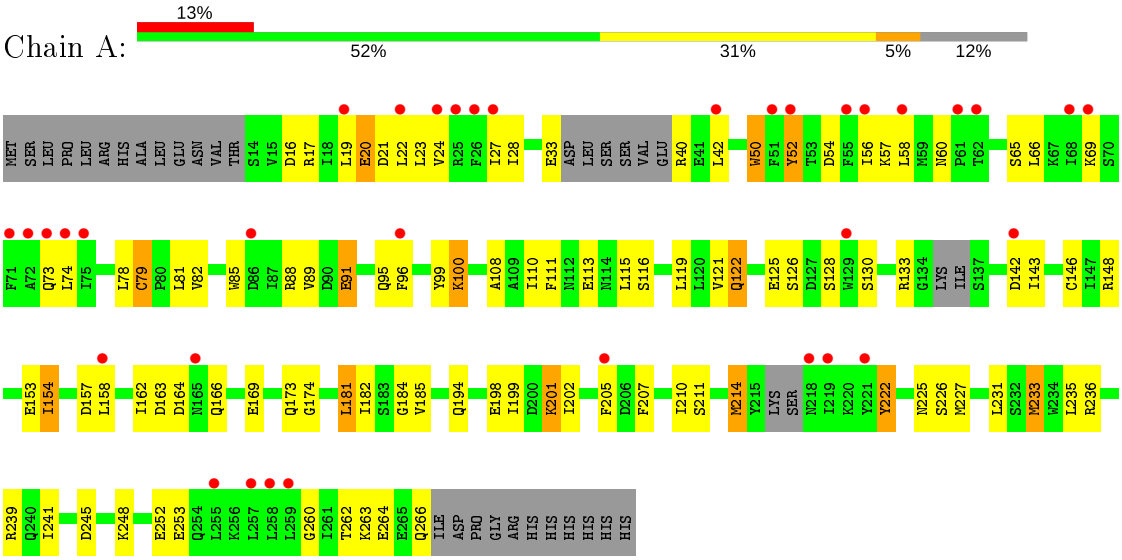
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	P	1	Total	Mg	0	0
			1	1		

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.

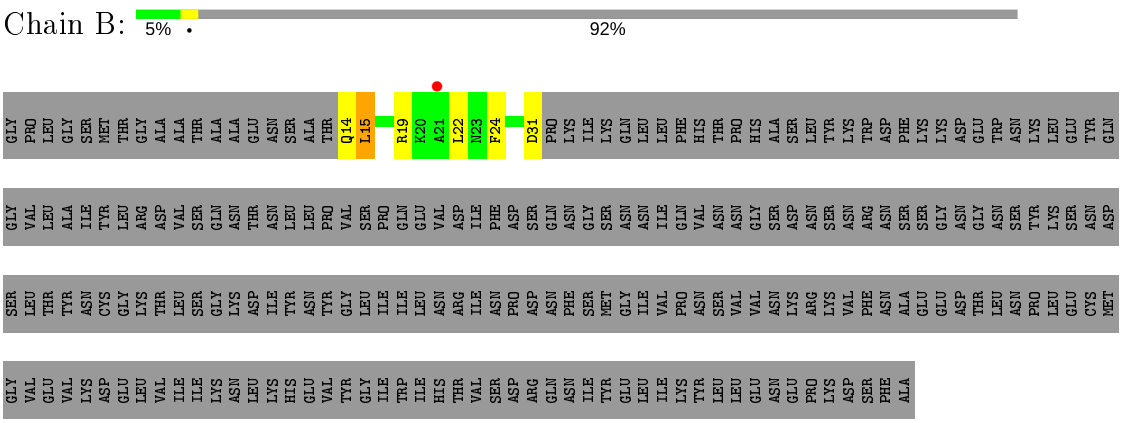
- Molecule 1: m7GpppN-mRNA hydrolase

Chain A:



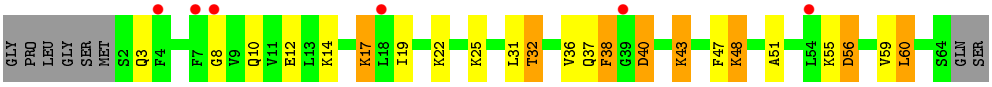
- Molecule 2: mRNA-decapping enzyme subunit 1

Chain B:

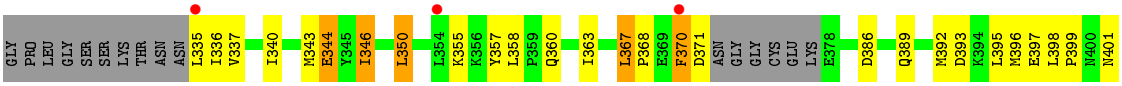


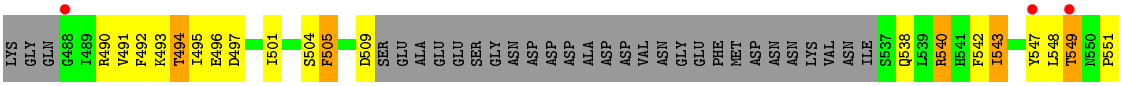
- Molecule 3: Enhancer of mRNA-decapping protein 3

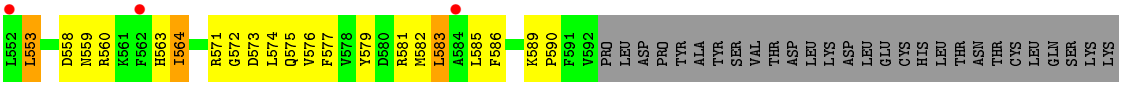
Chain C:

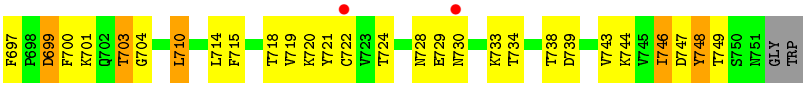


• Molecule 4: Probable tubulin–tyrosine ligase PBY1









4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	71.21Å 90.60Å 194.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.50 – 3.49 48.50 – 3.49	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.50-3.49) 99.5 (48.50-3.49)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	1.15 (at 3.48Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.246 , 0.321 0.274 , 0.368	Depositor DCC
R_{free} test set	767 reflections (4.64%)	wwPDB-VP
Wilson B-factor (Å^2)	145.9	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 181.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	5570	wwPDB-VP
Average B, all atoms (Å^2)	193.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.46	0/2086	0.71	0/2804
2	B	0.42	0/162	0.61	0/216
3	C	0.43	0/473	0.79	0/629
4	P	0.54	0/2961	0.83	0/4011
All	All	0.50	0/5682	0.78	0/7660

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

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	2044	0	2050	38	0
2	B	159	0	154	2	0
3	C	470	0	503	18	0
4	P	2896	0	2804	77	0
5	P	1	0	0	0	0
All	All	5570	0	5511	130	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 12.

All (130) 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)
4:P:585:LEU:HD23	4:P:627:VAL:HG12	1.53	0.90
3:C:19:ILE:CG2	3:C:36:VAL:CG2	2.57	0.82
3:C:19:ILE:CG2	3:C:36:VAL:HG22	2.10	0.81
1:A:252:GLU:HG2	3:C:59:VAL:HG12	1.62	0.81
1:A:88:ARG:HB3	1:A:91:GLU:HB3	1.64	0.79
1:A:113:GLU:HA	1:A:184:GLY:HA2	1.67	0.76
4:P:564:ILE:HD11	4:P:683:ILE:HG13	1.67	0.75
4:P:492:PHE:HB2	4:P:497:ASP:HB3	1.71	0.71
3:C:10:GLN:HB2	3:C:60:LEU:HD12	1.73	0.70
3:C:19:ILE:HG23	3:C:36:VAL:HG22	1.74	0.69
3:C:36:VAL:HG11	3:C:47:PHE:HB2	1.78	0.65
4:P:718:THR:O	4:P:722:CYS:HB2	1.97	0.64
4:P:563:HIS:HB2	4:P:682:LEU:HD23	1.80	0.64
4:P:453:LEU:O	4:P:457:LEU:HB2	1.98	0.64
4:P:439:TYR:CE2	4:P:441:GLU:HA	2.32	0.63
4:P:337:VAL:HG11	4:P:367:LEU:HB3	1.81	0.63
1:A:154:ILE:HG13	1:A:202:ILE:HD13	1.81	0.62
1:A:100:LYS:HE2	1:A:174:GLY:HA2	1.80	0.62
1:A:153:GLU:HB3	1:A:199:ILE:HG13	1.81	0.62
4:P:679:VAL:HG22	4:P:694:ILE:HG12	1.81	0.62
4:P:478:VAL:HG22	4:P:492:PHE:HE1	1.66	0.60
1:A:130:SER:HB3	1:A:222:TYR:HB3	1.83	0.60
4:P:585:LEU:CD2	4:P:627:VAL:HG12	2.28	0.59
4:P:715:PHE:O	4:P:719:VAL:HG23	2.05	0.57
4:P:406:SER:HA	4:P:675:GLU:HG2	1.85	0.57
4:P:427:THR:HG21	4:P:436:LYS:HB3	1.86	0.56
4:P:700:PHE:O	4:P:703:THR:HG23	2.05	0.56
4:P:654:ASP:O	4:P:658:ALA:HB2	2.05	0.56
1:A:122:GLN:HB3	1:A:201:LYS:HG3	1.87	0.56
4:P:412:ALA:HB2	4:P:666:ASN:HB3	1.88	0.56
4:P:392:MET:HG3	4:P:408:ILE:HD13	1.88	0.55
1:A:205:PHE:HB3	1:A:210:ILE:HD11	1.87	0.55
1:A:28:ILE:HD12	2:B:19:ARG:HD3	1.89	0.55
4:P:439:TYR:HE2	4:P:441:GLU:HA	1.72	0.55
3:C:19:ILE:HG22	3:C:36:VAL:CG2	2.36	0.54
4:P:494:THR:HB	4:P:497:ASP:H	1.73	0.54
3:C:12:GLU:HB2	3:C:56:ASP:HB2	1.90	0.54
4:P:444:THR:HG22	4:P:543:ILE:HD11	1.90	0.54
4:P:576:VAL:HB	4:P:746:ILE:HB	1.90	0.54
3:C:37:GLN:HG3	3:C:43:LYS:HE2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:579:TYR:CE2	4:P:714:LEU:HB2	2.44	0.53
1:A:111:PHE:HZ	1:A:231:LEU:HG	1.74	0.53
4:P:582:MET:HG3	4:P:630:PHE:CD1	2.44	0.53
1:A:108:ALA:HB2	1:A:146:CYS:SG	2.49	0.53
4:P:681:PHE:HA	4:P:691:LEU:HA	1.91	0.52
4:P:549:THR:C	4:P:551:PRO:HD3	2.30	0.52
1:A:42:LEU:HD13	1:A:96:PHE:HB2	1.92	0.52
4:P:357:TYR:CE1	4:P:720:LYS:HG3	2.44	0.52
1:A:50:TRP:HA	1:A:50:TRP:CE3	2.44	0.51
4:P:403:PHE:HA	4:P:672:ASN:O	2.11	0.51
4:P:585:LEU:HD23	4:P:627:VAL:CG1	2.33	0.51
3:C:19:ILE:HG21	3:C:36:VAL:CG2	2.40	0.50
4:P:479:LYS:HB2	4:P:543:ILE:HG22	1.93	0.50
1:A:52:TYR:OH	1:A:66:LEU:HB2	2.12	0.50
1:A:115:LEU:HD23	1:A:235:LEU:HD22	1.94	0.50
1:A:21:ASP:O	1:A:24:VAL:HG22	2.12	0.49
4:P:575:GLN:HG2	4:P:744:LYS:HE2	1.94	0.49
4:P:474:LYS:HE2	4:P:548:LEU:HD13	1.94	0.49
1:A:121:VAL:HG12	1:A:202:ILE:HG12	1.94	0.49
4:P:444:THR:HG22	4:P:543:ILE:CD1	2.42	0.49
1:A:58:LEU:HD13	1:A:233:MET:HB3	1.94	0.49
4:P:397:GLU:O	4:P:399:PRO:HD3	2.12	0.49
4:P:358:LEU:HD21	4:P:724:THR:HA	1.95	0.48
1:A:207:PHE:HA	1:A:210:ILE:HD12	1.96	0.48
4:P:398:LEU:HB3	4:P:401:ASN:HB2	1.96	0.48
1:A:162:ILE:HD12	1:A:182:ILE:HD11	1.96	0.48
1:A:20:GLU:O	1:A:23:LEU:HG	2.14	0.48
4:P:337:VAL:CG1	4:P:367:LEU:HB3	2.42	0.48
4:P:560:ARG:HA	4:P:590:PRO:HA	1.95	0.48
4:P:682:LEU:HD11	4:P:692:LEU:HD21	1.95	0.48
1:A:227:MET:O	1:A:231:LEU:HB2	2.14	0.47
4:P:657:LEU:HA	4:P:660:VAL:HG22	1.96	0.47
4:P:474:LYS:HD3	4:P:548:LEU:HB2	1.96	0.47
4:P:586:PHE:CD1	4:P:586:PHE:N	2.82	0.47
4:P:571:ARG:HD3	4:P:721:TYR:O	2.14	0.47
4:P:367:LEU:HD13	4:P:368:PRO:HD3	1.97	0.47
3:C:32:THR:HG23	3:C:48:LYS:HG3	1.96	0.46
4:P:579:TYR:CZ	4:P:581:ARG:HB2	2.50	0.46
4:P:457:LEU:HB3	4:P:464:ARG:HH21	1.80	0.46
1:A:50:TRP:HE3	1:A:50:TRP:HA	1.80	0.46
4:P:465:GLN:HA	4:P:468:GLU:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:586:PHE:CE1	4:P:628:LEU:HD12	2.50	0.46
4:P:686:ASN:HB2	4:P:688:GLU:OE1	2.16	0.46
1:A:166:GLN:HB3	1:A:181:LEU:HD12	1.98	0.46
4:P:699:ASP:HB2	4:P:701:LYS:HD2	1.98	0.46
1:A:57:LYS:HD3	1:A:65:SER:HB3	1.98	0.45
4:P:425:THR:O	4:P:429:LYS:HD2	2.17	0.45
4:P:449:TYR:HB3	4:P:540:ARG:NH2	2.31	0.45
4:P:406:SER:HA	4:P:675:GLU:CG	2.46	0.45
1:A:173:GLN:HA	4:P:368:PRO:HG3	1.99	0.45
4:P:478:VAL:HG22	4:P:492:PHE:CE1	2.48	0.45
1:A:73:GLN:HG3	1:A:89:VAL:HG21	1.99	0.45
1:A:50:TRP:CZ2	1:A:169:GLU:HB3	2.52	0.45
1:A:19:LEU:HA	1:A:22:LEU:HD12	1.99	0.45
4:P:579:TYR:CE1	4:P:581:ARG:HB2	2.52	0.44
3:C:17:LYS:HG3	3:C:40:ASP:OD2	2.18	0.44
4:P:501:ILE:HG22	4:P:505:PHE:HE2	1.83	0.44
4:P:340:ILE:HD11	4:P:344:GLU:HG3	1.99	0.44
4:P:572:GLY:HA2	4:P:670:LEU:O	2.18	0.44
3:C:19:ILE:HG22	3:C:36:VAL:HG23	1.99	0.44
3:C:36:VAL:HG13	3:C:38:PHE:CE1	2.54	0.43
1:A:248:LYS:O	3:C:59:VAL:HG11	2.18	0.43
4:P:346:ILE:O	4:P:350:LEU:HB3	2.19	0.43
4:P:457:LEU:HB3	4:P:464:ARG:NH2	2.34	0.43
4:P:577:PHE:HA	4:P:743:VAL:O	2.19	0.43
1:A:260:GLY:HA3	3:C:51:ALA:HB1	1.99	0.43
3:C:14:LYS:HG2	3:C:14:LYS:H	1.63	0.43
4:P:367:LEU:HB2	4:P:370:PHE:CZ	2.54	0.43
4:P:443:PHE:CZ	4:P:466:GLU:HG3	2.54	0.42
4:P:582:MET:HG3	4:P:630:PHE:HD1	1.82	0.42
4:P:748:TYR:HD1	4:P:749:THR:H	1.67	0.42
1:A:231:LEU:HA	1:A:231:LEU:HD12	1.90	0.42
4:P:645:LYS:HA	4:P:648:ILE:HD12	2.01	0.42
3:C:8:GLY:HA2	3:C:22:LYS:HA	2.02	0.42
4:P:553:LEU:HB3	4:P:559:ASN:HB3	2.02	0.42
4:P:583:LEU:CD2	4:P:710:LEU:HG	2.49	0.42
4:P:573:ASP:HA	4:P:574:LEU:HB2	2.01	0.42
1:A:119:LEU:HD11	1:A:202:ILE:HG22	2.01	0.42
1:A:79:CYS:O	1:A:82:VAL:HG22	2.20	0.42
1:A:205:PHE:CB	1:A:210:ILE:HD11	2.50	0.41
4:P:445:ILE:HG13	4:P:542:PHE:HB2	2.01	0.41
2:B:15:LEU:H	2:B:15:LEU:HD13	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:668:GLN:HA	4:P:669:PRO:HD3	1.89	0.41
1:A:110:ILE:HG23	1:A:185:VAL:HG21	2.02	0.41
4:P:682:LEU:CD2	4:P:692:LEU:HD11	2.49	0.41
4:P:720:LYS:HD2	4:P:721:TYR:CE1	2.56	0.41
4:P:386:ASP:HA	4:P:697:PHE:HE2	1.85	0.41
1:A:143:ILE:HG23	1:A:162:ILE:HG12	2.03	0.40
4:P:435:LEU:HD21	4:P:655:VAL:HB	2.03	0.40
4:P:412:ALA:HB3	4:P:667:PHE:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	235/277 (85%)	214 (91%)	17 (7%)	4 (2%)	9 42
2	B	16/236 (7%)	15 (94%)	1 (6%)	0	100 100
3	C	61/71 (86%)	53 (87%)	8 (13%)	0	100 100
4	P	338/429 (79%)	295 (87%)	38 (11%)	5 (2%)	10 45
All	All	650/1013 (64%)	577 (89%)	64 (10%)	9 (1%)	11 46

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	P	704	GLY
1	A	158	LEU
1	A	214	MET
4	P	346	ILE
4	P	505	PHE
4	P	625	SER
1	A	222	TYR

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Mol	Chain	Res	Type
4	P	662	VAL
1	A	263	LYS

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	230/262 (88%)	180 (78%)	50 (22%)	1	5
2	B	16/211 (8%)	11 (69%)	5 (31%)	0	2
3	C	50/56 (89%)	38 (76%)	12 (24%)	0	4
4	P	327/398 (82%)	250 (76%)	77 (24%)	1	4
All	All	623/927 (67%)	479 (77%)	144 (23%)	1	4

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ASP
1	A	17	ARG
1	A	20	GLU
1	A	27	ILE
1	A	33	GLU
1	A	40	ARG
1	A	50	TRP
1	A	52	TYR
1	A	54	ASP
1	A	56	ILE
1	A	60	ASN
1	A	69	LYS
1	A	74	LEU
1	A	78	LEU
1	A	79	CYS
1	A	81	LEU
1	A	85	TRP
1	A	91	GLU
1	A	95	GLN

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Mol	Chain	Res	Type
1	A	99	TYR
1	A	100	LYS
1	A	116	SER
1	A	122	GLN
1	A	125	GLU
1	A	126	SER
1	A	128	SER
1	A	133	ARG
1	A	142	ASP
1	A	148	ARG
1	A	154	ILE
1	A	157	ASP
1	A	163	ASP
1	A	164	ASP
1	A	181	LEU
1	A	194	GLN
1	A	198	GLU
1	A	201	LYS
1	A	211	SER
1	A	214	MET
1	A	225	ASN
1	A	226	SER
1	A	233	MET
1	A	236	ARG
1	A	239	ARG
1	A	241	ILE
1	A	245	ASP
1	A	253	GLU
1	A	262	THR
1	A	264	GLU
1	A	266	GLN
2	B	14	GLN
2	B	15	LEU
2	B	22	LEU
2	B	24	PHE
2	B	31	ASP
3	C	3	GLN
3	C	17	LYS
3	C	25	LYS
3	C	31	LEU
3	C	32	THR
3	C	38	PHE

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Mol	Chain	Res	Type
3	C	40	ASP
3	C	43	LYS
3	C	48	LYS
3	C	55	LYS
3	C	56	ASP
3	C	60	LEU
4	P	335	LEU
4	P	336	ILE
4	P	343	MET
4	P	344	GLU
4	P	350	LEU
4	P	355	LYS
4	P	360	GLN
4	P	363	ILE
4	P	367	LEU
4	P	370	PHE
4	P	371	ASP
4	P	389	GLN
4	P	393	ASP
4	P	395	LEU
4	P	396	MET
4	P	404	THR
4	P	410	ARG
4	P	411	LYS
4	P	415	ARG
4	P	416	LYS
4	P	420	SER
4	P	424	GLN
4	P	429	LYS
4	P	445	ILE
4	P	446	ASP
4	P	453	LEU
4	P	454	ASP
4	P	457	LEU
4	P	468	GLU
4	P	469	ASN
4	P	473	ASP
4	P	478	VAL
4	P	490	ARG
4	P	491	VAL
4	P	493	LYS
4	P	494	THR

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Mol	Chain	Res	Type
4	P	495	ILE
4	P	496	GLU
4	P	504	SER
4	P	509	ASP
4	P	538	GLN
4	P	540	ARG
4	P	543	ILE
4	P	547	TYR
4	P	549	THR
4	P	553	LEU
4	P	558	ASP
4	P	564	ILE
4	P	583	LEU
4	P	589	LYS
4	P	630	PHE
4	P	631	ASP
4	P	639	GLU
4	P	643	ASN
4	P	644	ILE
4	P	657	LEU
4	P	665	LEU
4	P	668	GLN
4	P	675	GLU
4	P	682	LEU
4	P	684	ASP
4	P	691	LEU
4	P	692	LEU
4	P	695	ASN
4	P	699	ASP
4	P	703	THR
4	P	710	LEU
4	P	728	ASN
4	P	729	GLU
4	P	730	ASN
4	P	733	LYS
4	P	734	THR
4	P	738	THR
4	P	739	ASP
4	P	746	ILE
4	P	747	ASP
4	P	748	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	243	ASN
1	A	254	GLN
4	P	383	HIS
4	P	400	ASN
4	P	672	ASN
4	P	732	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	243/277 (87%)	0.64	35 (14%) 2 3	136, 231, 289, 296	0
2	B	18/236 (7%)	0.54	1 (5%) 24 22	254, 263, 276, 279	0
3	C	63/71 (88%)	0.26	6 (9%) 8 8	172, 214, 255, 264	0
4	P	348/429 (81%)	0.21	20 (5%) 23 21	90, 157, 219, 270	0
All	All	672/1013 (66%)	0.38	62 (9%) 9 9	90, 188, 279, 296	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	71	PHE	5.4
1	A	61	PRO	5.3
1	A	142	ASP	5.1
1	A	68	ILE	4.9
1	A	75	ILE	4.8
1	A	62	THR	4.6
1	A	52	TYR	4.4
1	A	22	LEU	4.3
1	A	96	PHE	4.2
1	A	42	LEU	4.2
3	C	7	PHE	4.0
1	A	55	PHE	3.9
1	A	72	ALA	3.8
1	A	73	GLN	3.7
1	A	86	ASP	3.7
1	A	255	LEU	3.6
1	A	69	LYS	3.6
4	P	552	LEU	3.6
4	P	488	GLY	3.3
1	A	24	VAL	3.3
1	A	218	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	25	ARG	3.3
1	A	219	ILE	3.1
1	A	19	LEU	3.1
1	A	56	ILE	3.1
1	A	158	LEU	3.1
4	P	547	TYR	3.0
1	A	26	PHE	3.0
4	P	549	THR	2.9
1	A	27	ILE	2.9
1	A	258	LEU	2.9
4	P	630	PHE	2.9
1	A	51	PHE	2.8
4	P	480	PRO	2.8
4	P	335	LEU	2.8
1	A	221	TYR	2.7
3	C	18	LEU	2.7
1	A	58	LEU	2.6
1	A	74	LEU	2.6
3	C	4	PHE	2.5
4	P	474	LYS	2.5
1	A	257	LEU	2.5
1	A	205	PHE	2.5
4	P	478	VAL	2.5
4	P	354	LEU	2.4
4	P	562	PHE	2.3
4	P	479	LYS	2.3
4	P	426	TYR	2.3
4	P	722	CYS	2.2
4	P	481	SER	2.2
4	P	656	PHE	2.2
4	P	370	PHE	2.1
1	A	259	LEU	2.1
3	C	54	LEU	2.1
2	B	21	ALA	2.1
1	A	129	TRP	2.1
4	P	730	ASN	2.1
4	P	584	ALA	2.1
3	C	39	GLY	2.0
3	C	8	GLY	2.0
4	P	636	ILE	2.0
1	A	165	ASN	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 monosaccharides in this entry.

6.4 Ligands (i)

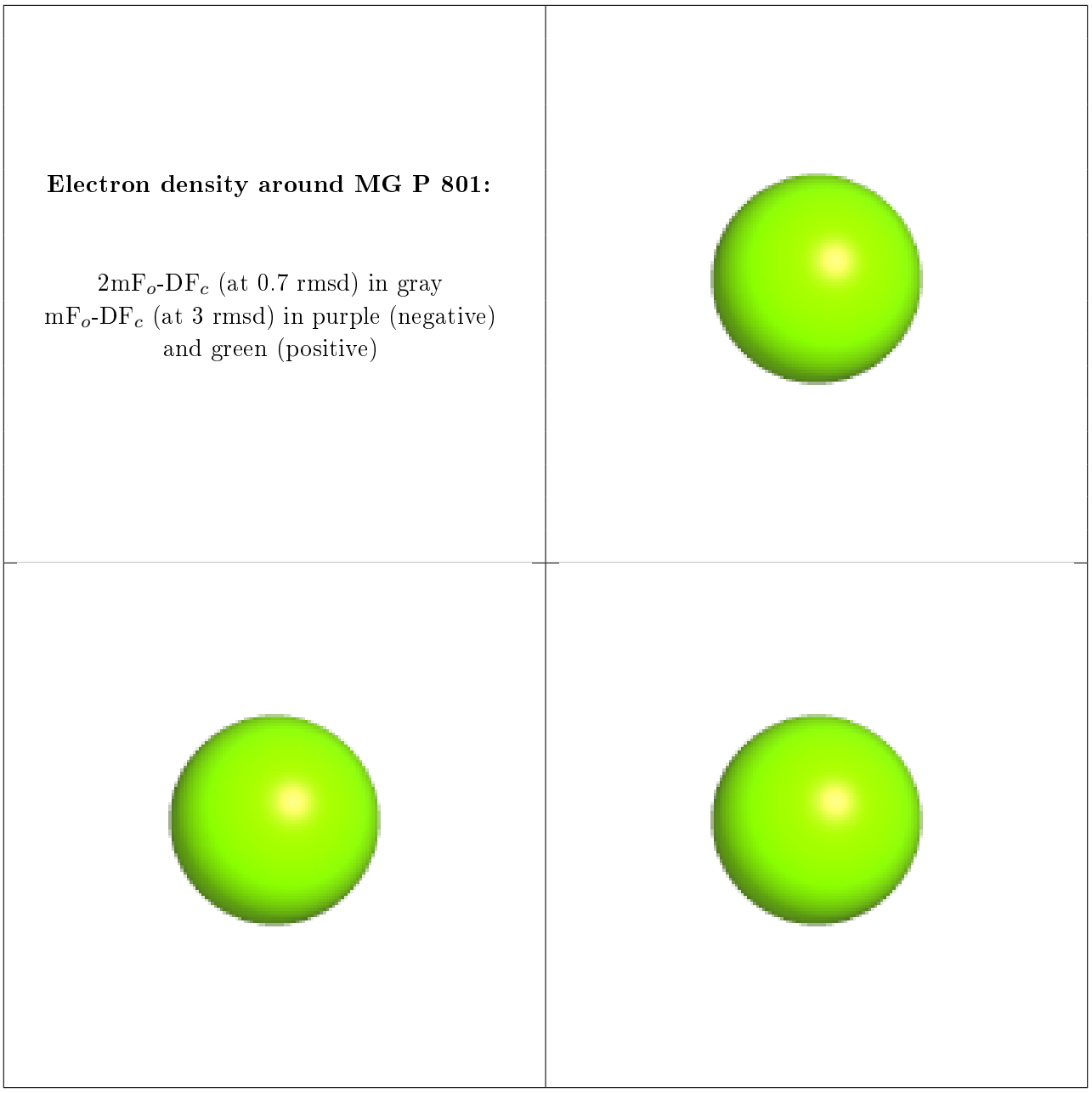
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MG	P	801	1/1	0.88	0.20	128,128,128,128	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 MG P 801:

$2mF_o$-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

There are no such residues in this entry.