Full wwPDB X-ray Structure Validation Report (i)

Sep 10, 2023 – 01:43 PM EDT

PDB ID	:	4JYC
Title	:	MeaB, A Bacterial Homolog of MMAA, in its Apo form
Authors	:	Koutmos, M.; Lofgren, M.; Padovani, D.; Banerjee, R.
Deposited on	:	2013-03-29
Resolution	:	2.20 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 (i) 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 (i)) were used in the production of this report:

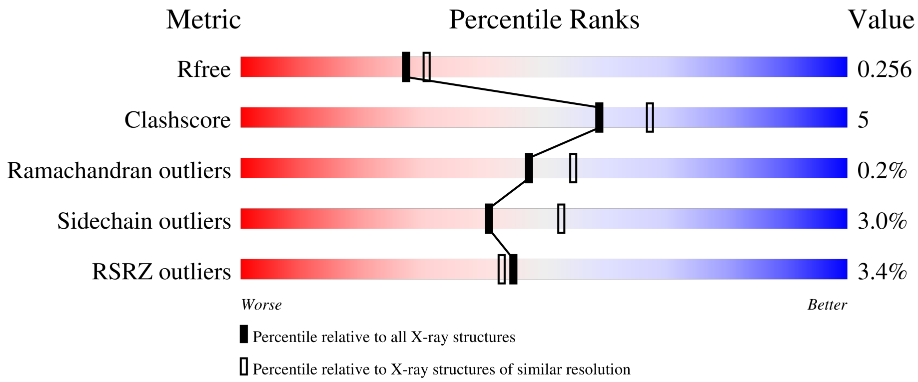
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

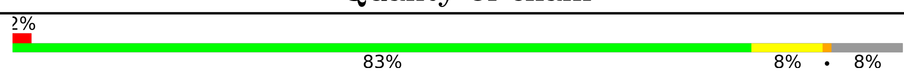
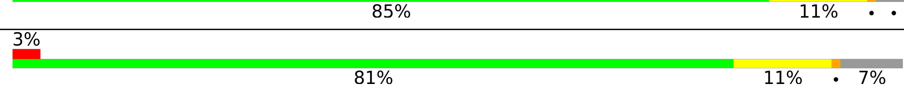
The reported resolution of this entry is 2.20 Å.

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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 <=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	337	 2% 83% 8% • 8%
1	B	337	 2% 83% 9% • 7%
1	C	337	 5% 85% 11% • •
1	D	337	 3% 81% 11% • 7%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 19474 atoms, of which 9646 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 Methylmalonyl-CoA mutase accessory protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	311	Total 4676	C 1433	H 2369	N 433	O 434	S 7	0	1	0
1	B	315	Total 4769	C 1460	H 2421	N 441	O 440	S 7	0	3	0
1	C	324	Total 4855	C 1488	H 2455	N 448	O 457	S 7	21	2	0
1	D	314	Total 4731	C 1452	H 2389	N 436	O 447	S 7	21	3	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	192	PHE	LEU	engineered mutation	UNP C5AP93
A	330	LEU	-	expression tag	UNP C5AP93
A	331	GLU	-	expression tag	UNP C5AP93
A	332	HIS	-	expression tag	UNP C5AP93
A	333	HIS	-	expression tag	UNP C5AP93
A	334	HIS	-	expression tag	UNP C5AP93
A	335	HIS	-	expression tag	UNP C5AP93
A	336	HIS	-	expression tag	UNP C5AP93
A	337	HIS	-	expression tag	UNP C5AP93
B	192	PHE	LEU	engineered mutation	UNP C5AP93
B	330	LEU	-	expression tag	UNP C5AP93
B	331	GLU	-	expression tag	UNP C5AP93
B	332	HIS	-	expression tag	UNP C5AP93
B	333	HIS	-	expression tag	UNP C5AP93
B	334	HIS	-	expression tag	UNP C5AP93
B	335	HIS	-	expression tag	UNP C5AP93
B	336	HIS	-	expression tag	UNP C5AP93
B	337	HIS	-	expression tag	UNP C5AP93
C	192	PHE	LEU	engineered mutation	UNP C5AP93
C	330	LEU	-	expression tag	UNP C5AP93
C	331	GLU	-	expression tag	UNP C5AP93

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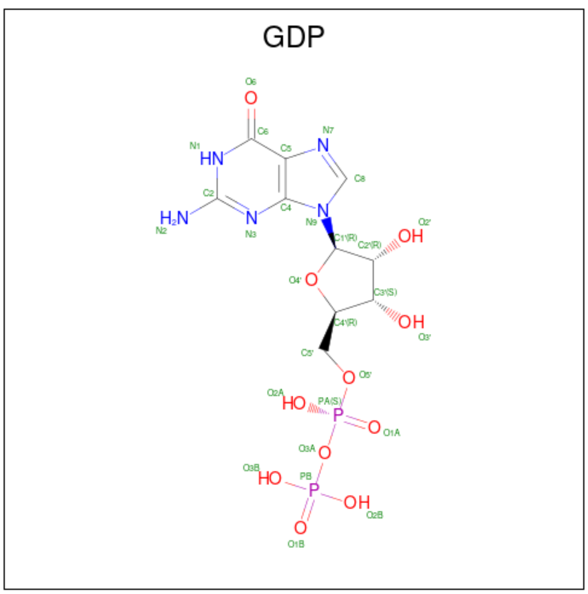
Chain	Residue	Modelled	Actual	Comment	Reference
C	332	HIS	-	expression tag	UNP C5AP93
C	333	HIS	-	expression tag	UNP C5AP93
C	334	HIS	-	expression tag	UNP C5AP93
C	335	HIS	-	expression tag	UNP C5AP93
C	336	HIS	-	expression tag	UNP C5AP93
C	337	HIS	-	expression tag	UNP C5AP93
D	192	PHE	LEU	engineered mutation	UNP C5AP93
D	330	LEU	-	expression tag	UNP C5AP93
D	331	GLU	-	expression tag	UNP C5AP93
D	332	HIS	-	expression tag	UNP C5AP93
D	333	HIS	-	expression tag	UNP C5AP93
D	334	HIS	-	expression tag	UNP C5AP93
D	335	HIS	-	expression tag	UNP C5AP93
D	336	HIS	-	expression tag	UNP C5AP93
D	337	HIS	-	expression tag	UNP C5AP93

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	P		
2	D	1	40	10	12	5	11	2	0	0

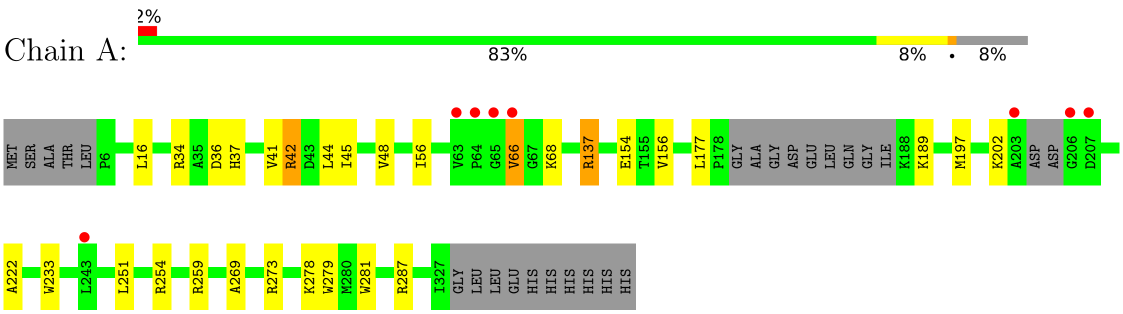
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	91	91	91	0	0
3	B	138	138	138	0	0
3	C	79	79	79	0	0
3	D	95	95	95	0	0

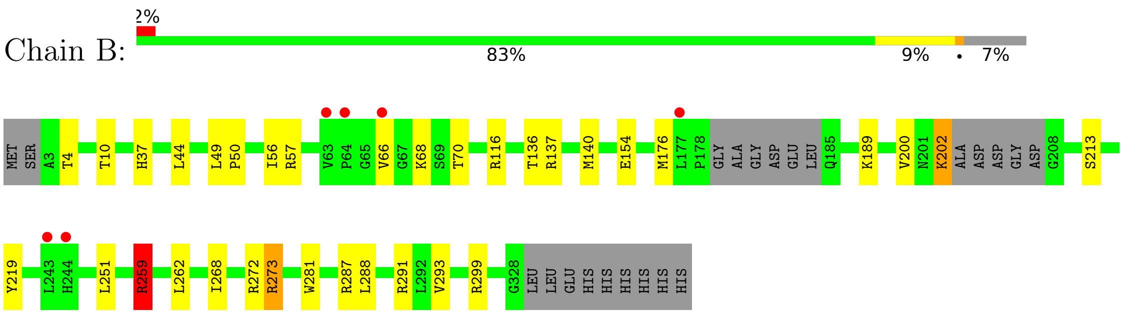
3 Residue-property plots ⓘ

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

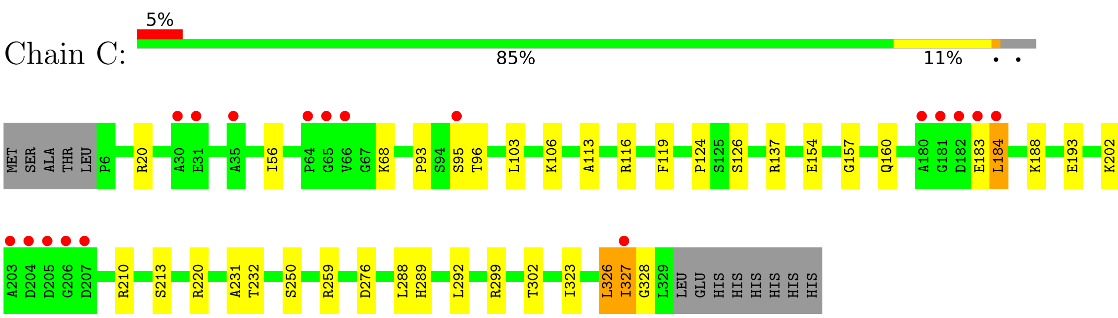
- Molecule 1: Methylmalonyl-CoA mutase accessory protein



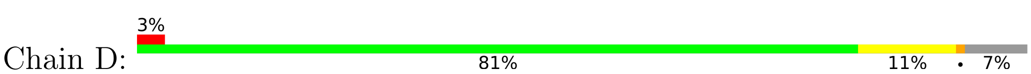
- Molecule 1: Methylmalonyl-CoA mutase accessory protein

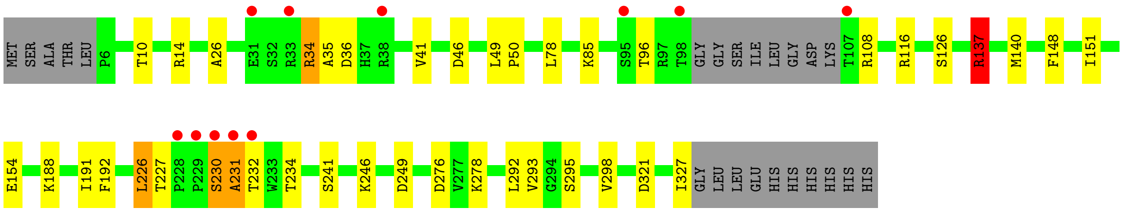


- Molecule 1: Methylmalonyl-CoA mutase accessory protein



- Molecule 1: Methylmalonyl-CoA mutase accessory protein




MET SER ALA THR LEU P6 T10 R14 A26 E31 S32 R33 R34 A35 D36 H37 R38 V41 D46 L49 P50 L78 K85 S95 T96 R97 T98 GLY GLY SER ILE LEU GLY ASP LYS T107 R108 R116 S126 R137 M140 F148 I151
E154 K188 I191 F192 L226 T227 P228 P229 S230 A231 T232 W233 T234 S241 K246 D249 D276 V277 K278 L292 V293 G294 S295 V298 D321 I327 GLY LEU LEU GLU HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	185.46Å 58.38Å 155.28Å 90.00° 110.07° 90.00°	Depositor
Resolution (Å)	48.62 – 2.20 48.62 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.0 (48.62-2.20) 97.0 (48.62-2.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.55 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.197 , 0.252 0.200 , 0.256	Depositor DCC
R_{free} test set	3932 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	32.4	Xtriage
Anisotropy	0.666	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 42.2	EDS
L-test for twinning[2]	$< \|L\| >$ = 0.48, $< L^2 >$ = 0.30	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	19474	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.94% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GDP

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	0.63	2/2341 (0.1%)	0.72	1/3169 (0.0%)
1	B	0.67	1/2388 (0.0%)	0.82	6/3233 (0.2%)
1	C	0.61	0/2439	0.71	0/3304
1	D	0.63	0/2383	0.77	2/3229 (0.1%)
All	All	0.63	3/9551 (0.0%)	0.75	9/12935 (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
1	A	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	281	TRP	CD2-CE2	5.55	1.48	1.41
1	B	281	TRP	CD2-CE2	5.36	1.47	1.41
1	A	233	TRP	CD2-CE2	5.18	1.47	1.41

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	137	ARG	NE-CZ-NH1	9.83	125.21	120.30
1	B	137	ARG	NE-CZ-NH1	8.24	124.42	120.30
1	D	137	ARG	NE-CZ-NH2	-7.74	116.43	120.30
1	B	273	ARG	NE-CZ-NH2	-7.02	116.79	120.30
1	A	137	ARG	NE-CZ-NH1	6.63	123.62	120.30
1	B	259	ARG	NE-CZ-NH1	6.49	123.54	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	259	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	B	137	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	B	273	ARG	NE-CZ-NH1	5.20	122.90	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	66	VAL	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	A	2307	2369	2369	21	0
1	B	2348	2421	2421	28	0
1	C	2400	2455	2455	23	0
1	D	2342	2389	2389	22	0
2	D	28	12	12	0	0
3	A	91	0	0	0	0
3	B	138	0	0	2	0
3	C	79	0	0	0	0
3	D	95	0	0	1	0
All	All	9828	9646	9646	89	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 5.

All (89) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116[A]:ARG:NH1	3:B:484:HOH:O	1.78	1.16
1:C:292:LEU:HD22	1:C:302:THR:HG21	1.51	0.92
1:C:327:ILE:HG22	1:C:328:GLY:H	1.43	0.82
1:B:4:THR:CG2	1:B:37:HIS:NE2	2.44	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:ARG:NH1	1:C:276:ASP:OD1	2.14	0.80
1:B:4:THR:HG23	1:B:37:HIS:NE2	1.96	0.80
1:B:176:MET:HE3	1:B:200:VAL:HG22	1.64	0.79
1:A:56:ILE:HG12	1:A:259[A]:ARG:HD2	1.64	0.78
1:B:176:MET:CE	1:B:200:VAL:HG22	2.13	0.78
1:D:10:THR:HG22	1:D:14[B]:ARG:HD3	1.70	0.71
1:C:96:THR:HA	1:C:126:SER:O	1.93	0.69
1:B:4:THR:HG21	1:B:37:HIS:NE2	2.11	0.66
1:C:292:LEU:HD22	1:C:302:THR:CG2	2.26	0.65
1:A:16:LEU:HD21	1:A:48:VAL:HG23	1.79	0.64
1:A:16:LEU:HD21	1:A:48:VAL:CG2	2.27	0.64
1:A:197:MET:HE3	1:A:254:ARG:HB2	1.85	0.59
1:C:231:ALA:HB1	1:C:232:THR:CA	2.32	0.58
1:B:189:LYS:O	1:C:193:GLU:OE1	2.22	0.58
1:A:68:LYS:HE3	1:A:154:GLU:OE2	2.03	0.58
1:C:231:ALA:HB1	1:C:232:THR:C	2.23	0.57
1:C:56:ILE:HG12	1:C:259:ARG:HD2	1.86	0.57
1:A:251:LEU:C	1:A:251:LEU:HD23	2.25	0.57
1:B:136:THR:O	1:B:140:MET:HG3	2.03	0.57
1:B:68:LYS:HD2	1:B:154:GLU:OE2	2.04	0.57
1:D:241:SER:HB3	1:D:246:LYS:HB2	1.87	0.56
1:C:183:GLU:HB3	1:C:184:LEU:HG	1.86	0.56
1:B:273:ARG:NH2	3:B:519:HOH:O	2.39	0.55
1:D:78:LEU:HD21	1:D:249:ASP:OD1	2.06	0.55
1:D:188:LYS:HB3	1:D:191:ILE:HD12	1.88	0.55
1:C:68:LYS:NZ	1:C:154:GLU:OE2	2.40	0.54
1:C:231:ALA:CB	1:C:232:THR:HA	2.38	0.53
1:D:96:THR:HA	1:D:126:SER:O	2.07	0.53
1:A:34:ARG:NH1	1:A:36:ASP:OD1	2.42	0.53
1:A:66:VAL:HB	1:A:177:LEU:HD21	1.91	0.52
1:C:231:ALA:CB	1:C:232:THR:CA	2.88	0.52
1:B:176:MET:CE	1:B:200:VAL:HG13	2.40	0.52
1:A:222:ALA:HB1	1:D:226:LEU:HD21	1.93	0.51
1:D:34:ARG:HB2	3:D:643:HOH:O	2.11	0.51
1:D:292:LEU:HD21	1:D:327:ILE:HD13	1.94	0.50
1:A:44:LEU:C	1:A:44:LEU:HD23	2.33	0.49
1:C:93:PRO:HD2	1:C:157:GLY:HA3	1.93	0.49
1:C:20:ARG:HD2	1:C:119:PHE:CD1	2.48	0.49
1:C:231:ALA:HB1	1:C:232:THR:HA	1.93	0.49
1:C:327:ILE:HG22	1:C:328:GLY:N	2.18	0.49
1:D:26:ALA:O	1:D:41:VAL:HG21	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:LYS:O	1:C:113:ALA:HB2	2.13	0.48
1:B:57:ARG:HD3	1:B:140:MET:HE1	1.95	0.48
1:B:293:VAL:HB	1:B:299:ARG:CZ	2.44	0.48
1:B:176:MET:HE2	1:B:219:TYR:HE2	1.79	0.48
1:B:262:LEU:HB3	1:B:268:ILE:HG13	1.96	0.47
1:C:323:ILE:O	1:C:326:LEU:HD22	2.14	0.47
1:C:160:GLN:HE22	1:C:188:LYS:HD3	1.79	0.47
1:D:10:THR:HG22	1:D:14[B]:ARG:CD	2.42	0.46
1:D:137:ARG:HD2	1:D:276:ASP:OD1	2.16	0.45
1:A:197:MET:HB2	1:A:197:MET:HE2	1.72	0.45
1:B:66:VAL:O	1:B:70:THR:HG23	2.16	0.45
1:B:176:MET:HE2	1:B:219:TYR:CE2	2.52	0.45
1:A:42:ARG:HA	1:A:42:ARG:HD3	1.73	0.45
1:B:176:MET:HE3	1:B:200:VAL:CG2	2.43	0.45
1:B:202:LYS:HG3	1:B:202:LYS:O	2.17	0.44
1:B:49:LEU:HB3	1:B:50:PRO:HD3	1.99	0.44
1:D:293:VAL:O	1:D:293:VAL:CG1	2.64	0.44
1:A:154:GLU:HG2	1:A:156:VAL:HG23	1.99	0.44
1:B:176:MET:HE3	1:B:200:VAL:HG13	1.98	0.44
1:D:85:LYS:HB2	1:D:148:PHE:HA	2.00	0.44
1:A:202:LYS:O	1:A:202:LYS:HD3	2.18	0.44
1:A:287:ARG:NH1	1:D:321:ASP:OD1	2.46	0.44
1:D:108:ARG:NH2	1:D:154:GLU:OE2	2.51	0.43
1:B:202:LYS:O	1:B:202:LYS:CG	2.67	0.43
1:D:140:MET:HG2	1:D:151:ILE:HG21	2.00	0.43
1:D:293:VAL:O	1:D:293:VAL:HG12	2.18	0.43
1:A:269:ALA:O	1:A:273:ARG:HG3	2.18	0.43
1:A:41:VAL:O	1:A:45:ILE:HD12	2.19	0.42
1:D:49:LEU:N	1:D:50:PRO:CD	2.82	0.42
1:B:44:LEU:HD23	1:B:44:LEU:C	2.40	0.42
1:B:288:LEU:HD22	1:C:288:LEU:HD22	2.01	0.42
1:B:251:LEU:C	1:B:251:LEU:HD23	2.40	0.42
1:D:35:ALA:O	1:D:36:ASP:HB3	2.20	0.42
1:D:230:SER:O	1:D:231:ALA:HB3	2.20	0.41
1:C:289:HIS:ND1	1:C:292:LEU:HD12	2.35	0.41
1:D:295:SER:OG	1:D:298:VAL:HG23	2.19	0.41
1:A:189:LYS:HB3	1:D:192:PHE:CE2	2.56	0.41
1:A:197:MET:CE	1:A:254:ARG:HB2	2.49	0.41
1:A:278:LYS:HE2	1:A:279:TRP:CH2	2.56	0.41
1:B:273:ARG:HA	1:B:273:ARG:HD3	1.86	0.41
1:B:56:ILE:HG12	1:B:259:ARG:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:ARG:HH22	1:B:272:ARG:NH2	2.19	0.41
1:A:41:VAL:O	1:A:41:VAL:HG22	2.21	0.40
1:C:95:SER:HB3	1:C:124:PRO:O	2.22	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	306/337 (91%)	300 (98%)	6 (2%)	0	100	100
1	B	312/337 (93%)	309 (99%)	3 (1%)	0	100	100
1	C	324/337 (96%)	308 (95%)	15 (5%)	1 (0%)	41	46
1	D	313/337 (93%)	305 (97%)	6 (2%)	2 (1%)	25	26
All	All	1255/1348 (93%)	1222 (97%)	30 (2%)	3 (0%)	47	55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	327	ILE
1	D	230	SER
1	D	231	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	A	234/253 (92%)	231 (99%)	3 (1%)	69	81
1	B	239/253 (94%)	233 (98%)	6 (2%)	47	60
1	C	243/253 (96%)	232 (96%)	11 (4%)	27	34
1	D	238/253 (94%)	229 (96%)	9 (4%)	33	42
All	All	954/1012 (94%)	925 (97%)	29 (3%)	41	53

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	HIS
1	A	42	ARG
1	A	137	ARG
1	B	10	THR
1	B	202	LYS
1	B	213	SER
1	B	259	ARG
1	B	287	ARG
1	B	291	ARG
1	C	103	LEU
1	C	116	ARG
1	C	184	LEU
1	C	202	LYS
1	C	210	ARG
1	C	213	SER
1	C	220[A]	ARG
1	C	220[B]	ARG
1	C	250	SER
1	C	299	ARG
1	C	326	LEU
1	D	34	ARG
1	D	46	ASP
1	D	116	ARG
1	D	137	ARG
1	D	226	LEU
1	D	227	THR
1	D	232	THR
1	D	234	THR
1	D	278	LYS

Sometimes 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 monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	GDP	D	501	-	24,30,30	0.97	2 (8%)	30,47,47	1.21	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
2	GDP	D	501	-	-	0/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	GDP	C6-N1	-2.63	1.34	1.37
2	D	501	GDP	C5-C4	2.02	1.48	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	GDP	C8-N7-C5	3.06	108.82	102.99
2	D	501	GDP	O4'-C4'-C3'	2.22	109.50	105.11
2	D	501	GDP	N2-C2-N3	-2.08	115.69	119.74

There are no chirality outliers.

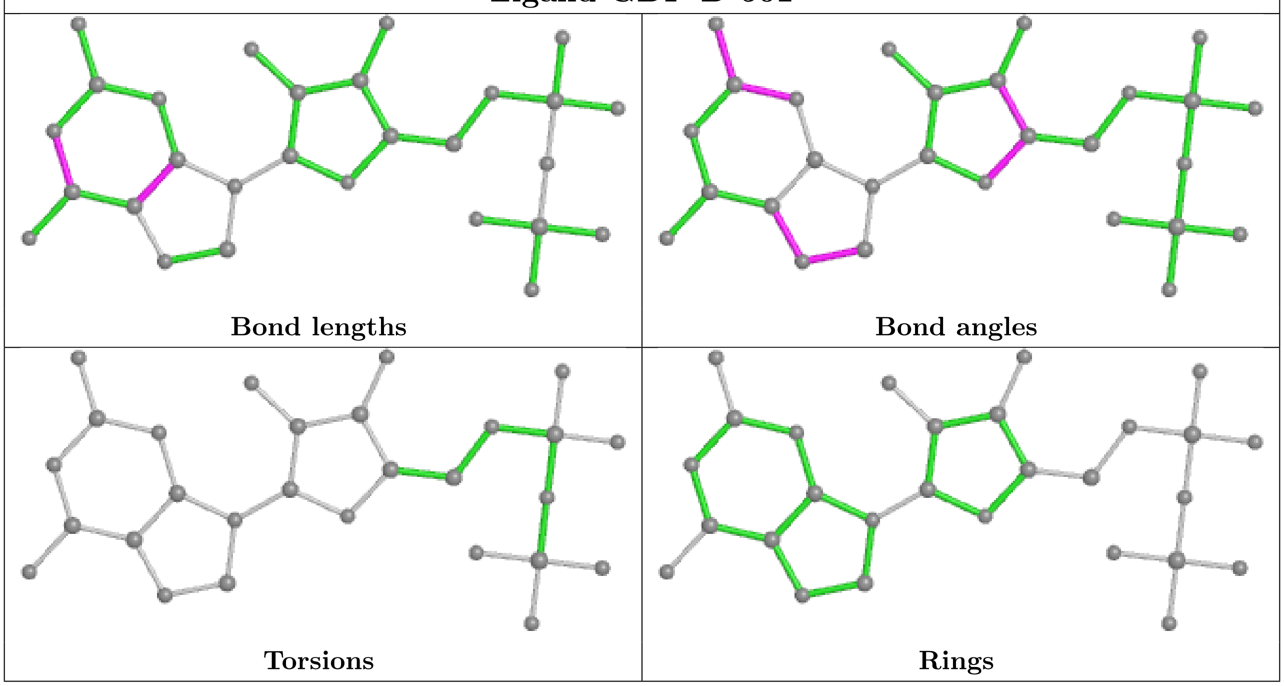
There are no torsion outliers.

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 then 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.

Ligand GDP D 501



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, 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	311/337 (92%)	-0.15	8 (2%)	56	53	24, 38, 63, 91	0
1	B	315/337 (93%)	-0.28	6 (1%)	66	65	20, 32, 59, 86	0
1	C	324/337 (96%)	0.10	18 (5%)	24	23	24, 39, 77, 123	0
1	D	314/337 (93%)	-0.12	11 (3%)	44	42	24, 36, 78, 107	0
All	All	1264/1348 (93%)	-0.11	43 (3%)	45	43	20, 36, 70, 123	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	182	ASP	8.5
1	A	64	PRO	7.0
1	C	206	GLY	6.7
1	C	183	GLU	6.6
1	D	33	ARG	6.1
1	D	229	PRO	5.7
1	C	203	ALA	5.7
1	D	228	PRO	5.5
1	A	66	VAL	5.3
1	C	66	VAL	5.1
1	C	180	ALA	4.3
1	C	181	GLY	4.1
1	C	184	LEU	3.9
1	C	204	ASP	3.9
1	C	205	ASP	3.6
1	C	65	GLY	3.4
1	D	230	SER	3.4
1	B	66	VAL	3.4
1	C	64	PRO	3.3
1	D	232	THR	3.3
1	A	65	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	231	ALA	3.1
1	B	177	LEU	3.0
1	C	30	ALA	2.9
1	A	243	LEU	2.9
1	A	206	GLY	2.8
1	D	31	GLU	2.7
1	C	31	GLU	2.6
1	B	244	HIS	2.6
1	C	207	ASP	2.6
1	D	107	THR	2.5
1	C	95	SER	2.5
1	B	243	LEU	2.4
1	D	95	SER	2.4
1	A	63	VAL	2.4
1	B	64	PRO	2.3
1	B	63	VAL	2.2
1	A	203	ALA	2.2
1	D	98	THR	2.2
1	D	38	ARG	2.2
1	C	327	ILE	2.1
1	C	35	ALA	2.0
1	A	207	ASP	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)

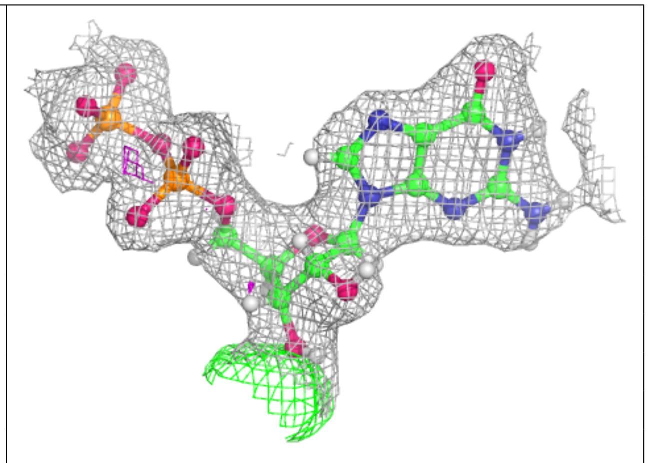
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

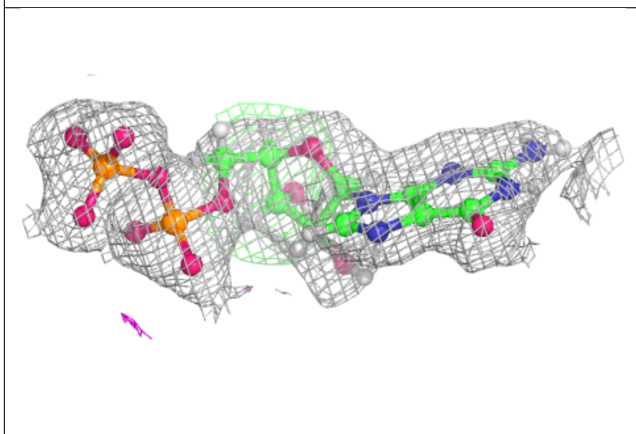
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
2	GDP	D	501	28/28	0.97	0.11	30,34,39,43	0

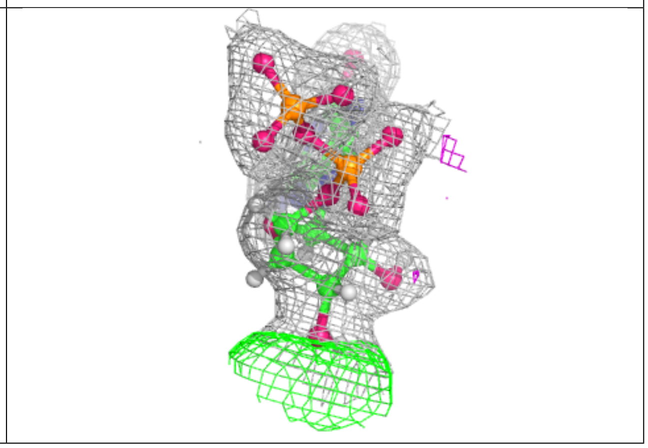
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around GDP D 501:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.