



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 10:17 am BST

PDB ID : 5YEW
Title : Structural basis for GTP hydrolysis and conformational change of mitofusin 1
in mediating mitochondrial fusion
Authors : Yan, L.; Qi, Y.; Huang, X.; Yu, C.
Deposited on : 2017-09-20
Resolution : 3.20 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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 : 2.11
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) : 2.11

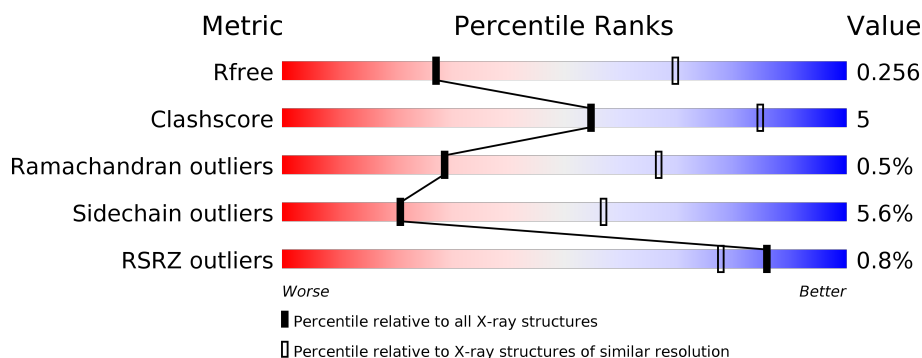
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 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 $\leq 5\%$. 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	421	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 16%, green 75%, grey 8%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 75% 16% • 7% </div> </div>
2	B	421	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 13%, green 76%, grey 9%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 76% 13% • 8% </div> </div>
2	C	421	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 79%, yellow 12%, grey 9%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 79% 12% • 8% </div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9431 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 Mitofusin-1,Mitofusin-1 fusion protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	0	0	0
			3121	1980	537	589	15			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	138	VAL	THR	engineered mutation	UNP Q8IWA4
A	139	ASN	VAL	engineered mutation	UNP Q8IWA4
A	685	GLY	-	linker	UNP Q8IWA4
A	686	SER	-	linker	UNP Q8IWA4
A	687	GLY	-	linker	UNP Q8IWA4
A	688	SER	-	linker	UNP Q8IWA4
A	689	GLY	-	linker	UNP Q8IWA4
A	690	SER	-	linker	UNP Q8IWA4
A	691	GLY	-	linker	UNP Q8IWA4
A	692	GLY	-	linker	UNP Q8IWA4
A	693	SER	-	linker	UNP Q8IWA4

- Molecule 2 is a protein called Mitofusin-1,Mitofusin-1 fusion protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	387	Total	C	N	O	S	0	0	0
			3094	1962	532	585	15			
2	C	389	Total	C	N	O	S	0	0	0
			3114	1975	535	589	15			

There are 18 discrepancies between the modelled and reference sequences:

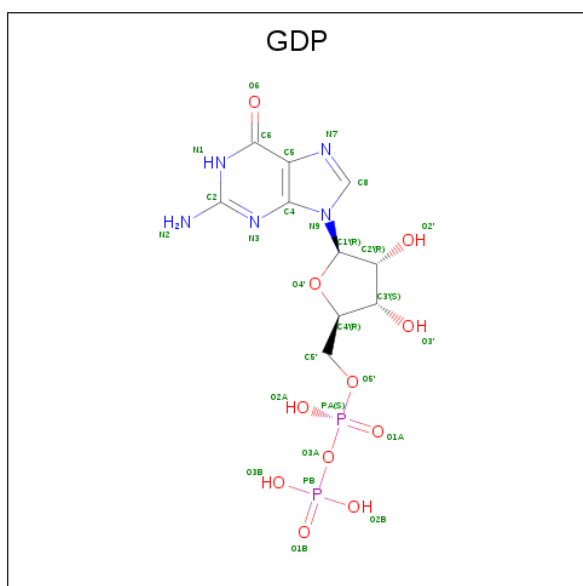
Chain	Residue	Modelled	Actual	Comment	Reference
B	685	GLY	-	linker	UNP Q8IWA4
B	686	SER	-	linker	UNP Q8IWA4
B	687	GLY	-	linker	UNP Q8IWA4

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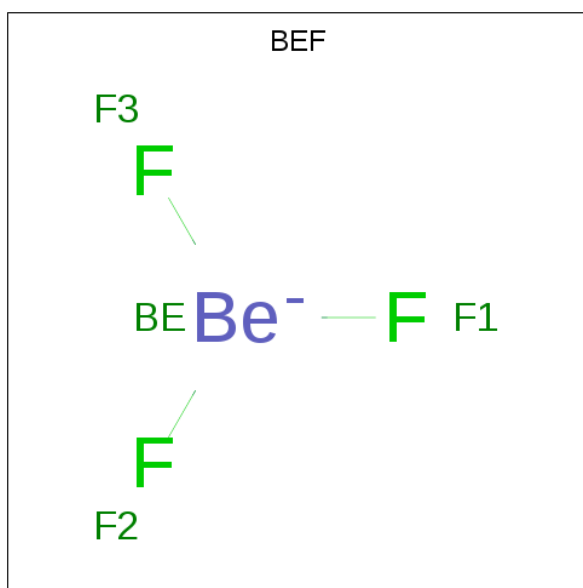
Chain	Residue	Modelled	Actual	Comment	Reference
B	688	SER	-	linker	UNP Q8IWA4
B	689	GLY	-	linker	UNP Q8IWA4
B	690	SER	-	linker	UNP Q8IWA4
B	691	GLY	-	linker	UNP Q8IWA4
B	692	GLY	-	linker	UNP Q8IWA4
B	693	SER	-	linker	UNP Q8IWA4
C	685	GLY	-	linker	UNP Q8IWA4
C	686	SER	-	linker	UNP Q8IWA4
C	687	GLY	-	linker	UNP Q8IWA4
C	688	SER	-	linker	UNP Q8IWA4
C	689	GLY	-	linker	UNP Q8IWA4
C	690	SER	-	linker	UNP Q8IWA4
C	691	GLY	-	linker	UNP Q8IWA4
C	692	GLY	-	linker	UNP Q8IWA4
C	693	SER	-	linker	UNP Q8IWA4

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 28	C 10	N 5	O 11	P 2	0	0
3	B	1	Total 28	C 10	N 5	O 11	P 2	0	0
3	C	1	Total 28	C 10	N 5	O 11	P 2	0	0

- Molecule 4 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Be	F	0	0
			4	1	3		
4	B	1	Total	Be	F	0	0
			4	1	3		
4	C	1	Total	Be	F	0	0
			4	1	3		

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	K	0	0
			1	1		
5	A	1	Total	K	0	0
			1	1		
5	C	1	Total	K	0	0
			1	1		

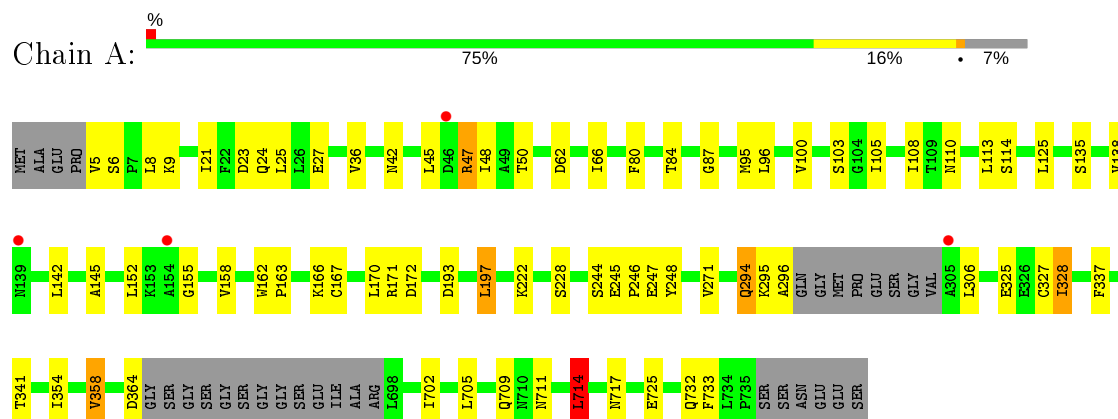
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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		

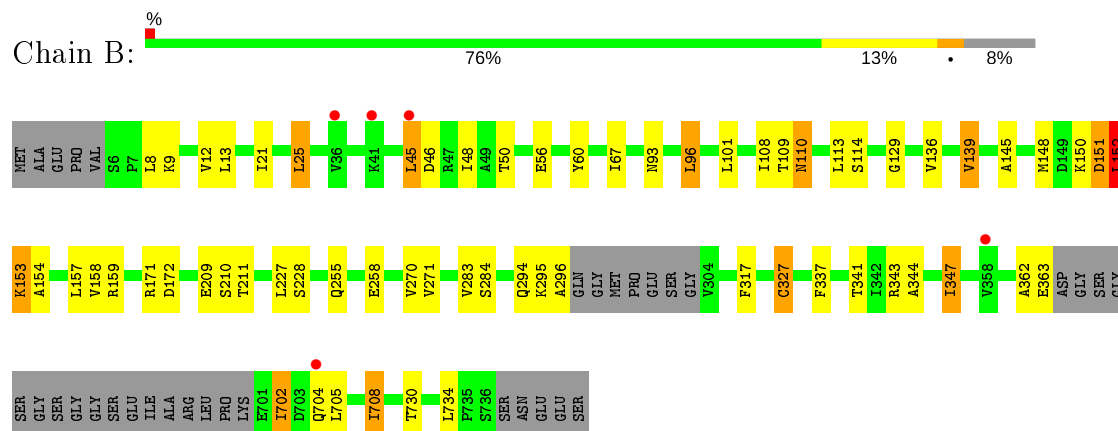
3 Residue-property plots [i](#)

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

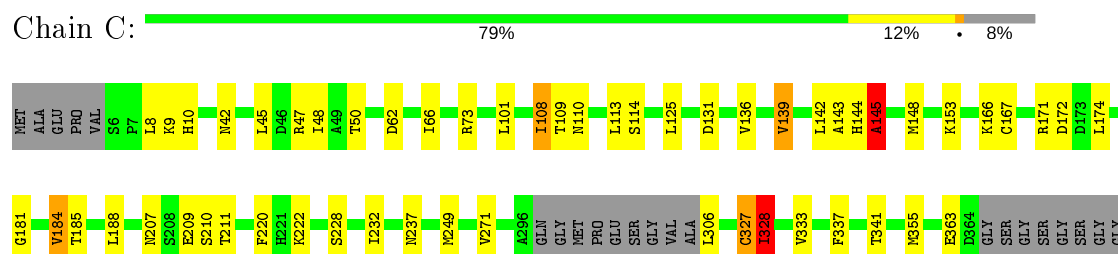
- Molecule 1: Mitofusin-1,Mitofusin-1 fusion protein



- Molecule 2: Mitofusin-1,Mitofusin-1 fusion protein



- Molecule 2: Mitofusin-1,Mitofusin-1 fusion protein



SER	GLU	ILE	ALA	ARG	L698	S712	S736	SER	ASN	GLU	GLU	SER
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4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	207.94Å 207.94Å 107.89Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.20 180.08 – 3.20	Depositor EDS
% Data completeness (in resolution range)	90.9 (50.00-3.20) 90.9 (180.08-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.223 , 0.257 0.222 , 0.256	Depositor DCC
R_{free} test set	1941 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	63.3	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 33.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.029 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9431	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, K, BEF, 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	0.44	0/3174	0.78	7/4275 (0.2%)
2	B	0.45	0/3146	0.83	8/4237 (0.2%)
2	C	0.43	0/3167	0.76	10/4265 (0.2%)
All	All	0.44	0/9487	0.79	25/12777 (0.2%)

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
2	B	0	1
2	C	0	2
All	All	0	4

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	45	LEU	CB-CA-C	-13.34	84.86	110.20
1	A	295	LYS	N-CA-CB	-12.91	87.36	110.60
2	C	167	CYS	N-CA-CB	-10.04	92.54	110.60
1	A	714	LEU	CA-CB-CG	9.63	137.45	115.30
1	A	294	GLN	N-CA-C	9.13	135.65	111.00
2	B	327	CYS	N-CA-C	8.29	133.37	111.00
1	A	294	GLN	CB-CA-C	-8.10	94.20	110.40
2	C	145	ALA	N-CA-C	-8.08	89.17	111.00
1	A	155	GLY	N-CA-C	-6.85	95.98	113.10
2	C	306	LEU	CA-CB-CG	6.79	130.91	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	152	LEU	CA-CB-CG	6.63	130.55	115.30
2	B	96	LEU	N-CA-C	-6.41	93.70	111.00
2	B	129	GLY	N-CA-C	-6.40	97.09	113.10
2	C	73	ARG	NE-CZ-NH2	-6.23	117.19	120.30
2	C	73	ARG	NE-CZ-NH1	6.22	123.41	120.30
2	B	228	SER	N-CA-CB	6.03	119.54	110.50
2	C	328	ILE	N-CA-CB	-5.96	97.09	110.80
2	C	145	ALA	C-N-CA	5.95	136.58	121.70
2	C	166	LYS	N-CA-C	5.79	126.63	111.00
2	C	327	CYS	N-CA-C	5.67	126.30	111.00
2	B	343	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	A	228	SER	N-CA-CB	5.35	118.53	110.50
2	C	228	SER	N-CA-CB	5.21	118.32	110.50
1	A	125	LEU	CA-CB-CG	5.10	127.03	115.30
2	B	152	LEU	CB-CG-CD1	5.01	119.52	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	152	LEU	Peptide
2	B	46	ASP	Peptide
2	C	145	ALA	Peptide
2	C	363	GLU	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	3121	0	3125	31	0
2	B	3094	0	3098	44	0
2	C	3114	0	3121	24	0
3	A	28	0	12	3	0
3	B	28	0	12	0	0
3	C	28	0	12	0	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	4	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
All	All	9431	0	9380	98	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 (98) 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:45:LEU:O	2:B:48:ILE:HD13	1.37	1.19
2:B:362:ALA:HB2	2:B:708:ILE:HD11	1.50	0.93
2:B:93:ASN:O	2:B:96:LEU:O	1.97	0.83
1:A:23:ASP:O	1:A:27:GLU:OE1	2.02	0.76
2:B:136:VAL:O	2:B:139:VAL:HG22	1.90	0.70
2:C:136:VAL:O	2:C:139:VAL:HG22	1.91	0.70
2:B:283:VAL:HG21	2:B:317:PHE:HD1	1.59	0.67
1:A:354:ILE:O	1:A:358:VAL:HG23	1.95	0.66
2:B:283:VAL:HG21	2:B:317:PHE:CD1	2.31	0.66
1:A:135:SER:O	1:A:138:VAL:HG22	1.96	0.65
2:C:207:ASN:OD1	2:C:209:GLU:HG2	1.96	0.64
2:B:148:MET:HB3	2:B:152:LEU:CD2	2.29	0.63
2:B:148:MET:HB3	2:B:152:LEU:HD23	1.81	0.62
2:B:705:LEU:O	2:B:708:ILE:HG13	2.01	0.60
2:B:67:ILE:HD11	2:B:227:LEU:O	2.02	0.60
3:A:801:GDP:O2A	3:A:801:GDP:O2B	2.21	0.59
2:C:143:ALA:C	2:C:148:MET:CE	2.71	0.59
2:B:151:ASP:HA	2:B:152:LEU:CB	2.33	0.59
2:B:45:LEU:HD21	2:B:704:GLN:HE21	1.68	0.58
1:A:294:GLN:O	1:A:296:ALA:N	2.35	0.58
2:C:144:HIS:N	2:C:148:MET:HE2	2.19	0.58
2:C:45:LEU:HD23	2:C:48:ILE:HG13	1.84	0.57
1:A:732:GLN:HG3	1:A:733:PHE:CD2	2.39	0.57
2:C:110:ASN:HD22	2:C:145:ALA:HB2	1.70	0.57
1:A:45:LEU:HD23	1:A:48:ILE:HG13	1.85	0.57
2:C:62:ASP:O	2:C:66:ILE:HD12	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:143:ALA:C	2:C:148:MET:HE2	2.25	0.56
1:A:62:ASP:O	1:A:66:ILE:HD12	2.06	0.55
2:B:362:ALA:O	2:B:705:LEU:HD21	2.06	0.55
2:C:125:LEU:HD13	2:C:136:VAL:HA	1.87	0.54
2:C:181:GLY:O	2:C:184:VAL:HG12	2.06	0.54
1:A:87:GLY:HA2	3:A:801:GDP:O2A	2.08	0.54
2:C:185:THR:HG23	2:C:188:LEU:HB2	1.89	0.54
2:C:174:LEU:HD13	2:C:328:ILE:HG13	1.90	0.53
1:A:110:ASN:HB2	1:A:145:ALA:HB2	1.91	0.53
2:B:152:LEU:CD1	2:B:153:LYS:HG2	2.39	0.52
2:B:21:ILE:HG22	2:B:25:LEU:HD23	1.91	0.52
1:A:105:ILE:HG23	2:B:209:GLU:HA	1.91	0.52
1:A:163:PRO:O	1:A:166:LYS:O	2.28	0.51
2:B:157:LEU:HD23	2:B:158:VAL:N	2.25	0.51
1:A:245:GLU:N	1:A:246:PRO:HD3	2.26	0.51
2:B:9:LYS:HA	2:B:12:VAL:HG22	1.91	0.51
1:A:714:LEU:O	1:A:717:ASN:OD1	2.28	0.50
2:B:270:VAL:HG13	2:B:271:VAL:HG22	1.94	0.50
1:A:167:CYS:SG	1:A:170:LEU:HD23	2.51	0.50
2:B:344:ALA:HA	2:B:347:ILE:HD11	1.93	0.50
1:A:5:VAL:HA	1:A:6:SER:HB3	1.93	0.50
2:B:151:ASP:HA	2:B:152:LEU:HG	1.93	0.50
2:C:110:ASN:HB3	2:C:148:MET:CE	2.42	0.49
1:A:100:VAL:HG21	1:A:162:TRP:CZ3	2.47	0.49
2:B:110:ASN:HB2	2:B:145:ALA:HB2	1.94	0.49
1:A:247:GLU:HG2	1:A:248:TYR:CD1	2.46	0.49
1:A:711:ASN:HA	1:A:714:LEU:HD22	1.95	0.49
2:B:255:GLN:O	2:B:258:GLU:HG2	2.13	0.48
1:A:21:ILE:CD1	1:A:725:GLU:HB3	2.44	0.47
2:B:60:TYR:CE1	2:B:347:ILE:HG22	2.48	0.47
2:B:344:ALA:O	2:B:347:ILE:HG12	2.15	0.47
2:B:157:LEU:HD22	2:B:159:ARG:HG3	1.95	0.47
2:B:702:ILE:HG23	2:B:705:LEU:HB3	1.96	0.47
2:B:294:GLN:O	2:B:294:GLN:HG2	2.15	0.47
2:B:295:LYS:H	2:B:296:ALA:HA	1.78	0.47
2:B:283:VAL:CG2	2:B:317:PHE:HB2	2.45	0.47
1:A:325:GLU:HA	1:A:328:ILE:CD1	2.45	0.46
2:B:283:VAL:HG22	2:B:284:SER:N	2.31	0.45
1:A:84:THR:HG21	2:B:211:THR:HG22	1.99	0.45
2:C:110:ASN:HB3	2:C:148:MET:HE3	1.98	0.45
1:A:80:PHE:HZ	1:A:95:MET:HE1	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:295:LYS:N	2:B:296:ALA:HA	2.33	0.44
1:A:711:ASN:O	1:A:714:LEU:HD22	2.18	0.44
2:B:101:LEU:HD22	2:B:113:LEU:HD22	1.99	0.44
2:B:337:PHE:O	2:B:341:THR:HG23	2.18	0.43
2:B:344:ALA:HA	2:B:347:ILE:CD1	2.47	0.43
1:A:113:LEU:HD23	1:A:158:VAL:HB	2.00	0.43
2:C:337:PHE:O	2:C:341:THR:HG23	2.18	0.43
2:B:283:VAL:HG21	2:B:317:PHE:HB2	1.99	0.43
2:B:151:ASP:HA	2:B:152:LEU:CG	2.48	0.43
2:C:185:THR:CG2	2:C:188:LEU:HD13	2.49	0.43
2:B:45:LEU:HB3	2:B:48:ILE:HD13	2.01	0.42
1:A:24:GLN:HA	1:A:27:GLU:OE1	2.19	0.42
2:C:355:MET:HE2	2:C:712:SER:HA	2.02	0.42
2:C:10:HIS:CD2	2:C:333:VAL:HG21	2.55	0.41
1:A:193:ASP:O	1:A:197:LEU:HB2	2.19	0.41
2:C:42:ASN:HB3	2:C:45:LEU:HD13	2.02	0.41
1:A:337:PHE:O	1:A:341:THR:HG23	2.19	0.41
2:B:730:THR:HG22	2:B:734:LEU:HD12	2.02	0.41
1:A:103:SER:HB2	3:A:801:GDP:O1A	2.20	0.41
2:B:45:LEU:O	2:B:48:ILE:CD1	2.32	0.41
2:C:237:ASN:CG	2:C:237:ASN:O	2.59	0.41
1:A:96:LEU:HD13	1:A:100:VAL:HG11	2.03	0.41
2:B:152:LEU:HD12	2:B:153:LYS:HG2	2.03	0.41
2:B:56:GLU:HG2	2:B:60:TYR:CE2	2.56	0.41
2:C:220:PHE:CD1	2:C:232:ILE:HD11	2.56	0.41
2:C:101:LEU:HD22	2:C:113:LEU:HD22	2.02	0.41
1:A:42:ASN:HB3	1:A:45:LEU:HD13	2.03	0.41
1:A:80:PHE:CZ	1:A:95:MET:HE1	2.56	0.41
2:C:210:SER:OG	2:C:211:THR:N	2.54	0.41
2:B:210:SER:OG	2:B:211:THR:N	2.54	0.40
2:C:108:ILE:HG22	2:C:109:THR:N	2.36	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	384/421 (91%)	366 (95%)	17 (4%)	1 (0%)	41	74
2	B	381/421 (90%)	359 (94%)	18 (5%)	4 (1%)	15	54
2	C	383/421 (91%)	367 (96%)	15 (4%)	1 (0%)	41	74
All	All	1148/1263 (91%)	1092 (95%)	50 (4%)	6 (0%)	29	67

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47	ARG
2	B	150	LYS
2	B	153	LYS
2	C	47	ARG
2	B	151	ASP
2	B	154	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	346/368 (94%)	322 (93%)	24 (7%)	15	49
2	B	343/368 (93%)	326 (95%)	17 (5%)	24	60
2	C	346/368 (94%)	329 (95%)	17 (5%)	25	61
All	All	1035/1104 (94%)	977 (94%)	58 (6%)	21	57

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	9	LYS
1	A	25	LEU
1	A	36	VAL

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Mol	Chain	Res	Type
1	A	47	ARG
1	A	50	THR
1	A	108	ILE
1	A	114	SER
1	A	142	LEU
1	A	171	ARG
1	A	172	ASP
1	A	197	LEU
1	A	222	LYS
1	A	244	SER
1	A	271	VAL
1	A	306	LEU
1	A	327	CYS
1	A	328	ILE
1	A	358	VAL
1	A	364	ASP
1	A	702	ILE
1	A	705	LEU
1	A	709	GLN
1	A	714	LEU
2	B	8	LEU
2	B	13	LEU
2	B	25	LEU
2	B	50	THR
2	B	108	ILE
2	B	109	THR
2	B	110	ASN
2	B	114	SER
2	B	139	VAL
2	B	152	LEU
2	B	171	ARG
2	B	172	ASP
2	B	327	CYS
2	B	347	ILE
2	B	363	GLU
2	B	702	ILE
2	B	708	ILE
2	C	8	LEU
2	C	9	LYS
2	C	50	THR
2	C	108	ILE
2	C	114	SER

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Mol	Chain	Res	Type
2	C	131	ASP
2	C	139	VAL
2	C	142	LEU
2	C	153	LYS
2	C	171	ARG
2	C	172	ASP
2	C	184	VAL
2	C	222	LYS
2	C	249	MET
2	C	271	VAL
2	C	327	CYS
2	C	328	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	294	GLN
2	B	294	GLN
2	B	359	ASN
2	B	704	GLN
2	B	709	GLN
2	C	10	HIS
2	C	110	ASN

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 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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	$\# Z > 2$
3	GDP	A	801	5,4,6	24,30,30	1.15	2 (8%)	31,47,47	1.95	8 (25%)
3	GDP	B	801	5,6	24,30,30	1.08	2 (8%)	31,47,47	2.02	9 (29%)
3	GDP	C	801	5,6	24,30,30	1.12	2 (8%)	31,47,47	1.87	9 (29%)
4	BEF	C	802	-	0,3,3	0.00	-	-		
4	BEF	B	802	-	0,3,3	0.00	-	-		
4	BEF	A	802	3	0,3,3	0.00	-	-		

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
3	GDP	A	801	5,4,6	-	8/12/32/32	0/3/3/3
3	GDP	B	801	5,6	-	0/12/32/32	0/3/3/3
3	GDP	C	801	5,6	-	4/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	801	GDP	C6-C5	4.02	1.48	1.41
3	C	801	GDP	C6-C5	3.91	1.48	1.41
3	B	801	GDP	C6-C5	3.77	1.47	1.41
3	A	801	GDP	C5-C4	2.40	1.47	1.40
3	C	801	GDP	C5-C4	2.29	1.47	1.40
3	B	801	GDP	C5-C4	2.22	1.46	1.40

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	801	GDP	C2-N3-C4	4.76	120.79	115.36
3	B	801	GDP	C6-C5-C4	-4.65	116.36	120.80
3	A	801	GDP	C2-N3-C4	4.60	120.61	115.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	801	GDP	C2-N3-C4	4.50	120.50	115.36
3	C	801	GDP	C6-C5-C4	-4.09	116.89	120.80
3	B	801	GDP	C6-N1-C2	4.03	122.34	115.93
3	A	801	GDP	C5-C6-N1	-3.95	118.02	123.43
3	B	801	GDP	C5-C6-N1	-3.83	118.20	123.43
3	A	801	GDP	C6-C5-C4	-3.69	117.27	120.80
3	A	801	GDP	C6-N1-C2	3.68	121.78	115.93
3	A	801	GDP	PA-O3A-PB	-3.52	120.74	132.83
3	C	801	GDP	C6-N1-C2	3.51	121.51	115.93
3	B	801	GDP	N3-C2-N1	-3.45	122.62	127.22
3	C	801	GDP	C5-C6-N1	-3.26	118.97	123.43
3	C	801	GDP	N3-C2-N1	-3.16	123.00	127.22
3	B	801	GDP	PA-O3A-PB	-3.07	122.29	132.83
3	A	801	GDP	N3-C2-N1	-3.01	123.21	127.22
3	C	801	GDP	PA-O3A-PB	-2.76	123.37	132.83
3	B	801	GDP	C1'-N9-C4	-2.47	122.31	126.64
3	C	801	GDP	C4-C5-N7	-2.29	107.01	109.40
3	B	801	GDP	C4-C5-N7	-2.22	107.09	109.40
3	A	801	GDP	C4-C5-N7	-2.21	107.10	109.40
3	B	801	GDP	O3B-PB-O2B	2.18	115.98	107.64
3	C	801	GDP	O3B-PB-O2B	2.16	115.90	107.64
3	C	801	GDP	O2A-PA-O1A	2.06	122.42	112.24
3	A	801	GDP	C1'-N9-C4	-2.00	123.12	126.64

There are no chirality outliers.

All (12) torsion outliers are listed below:

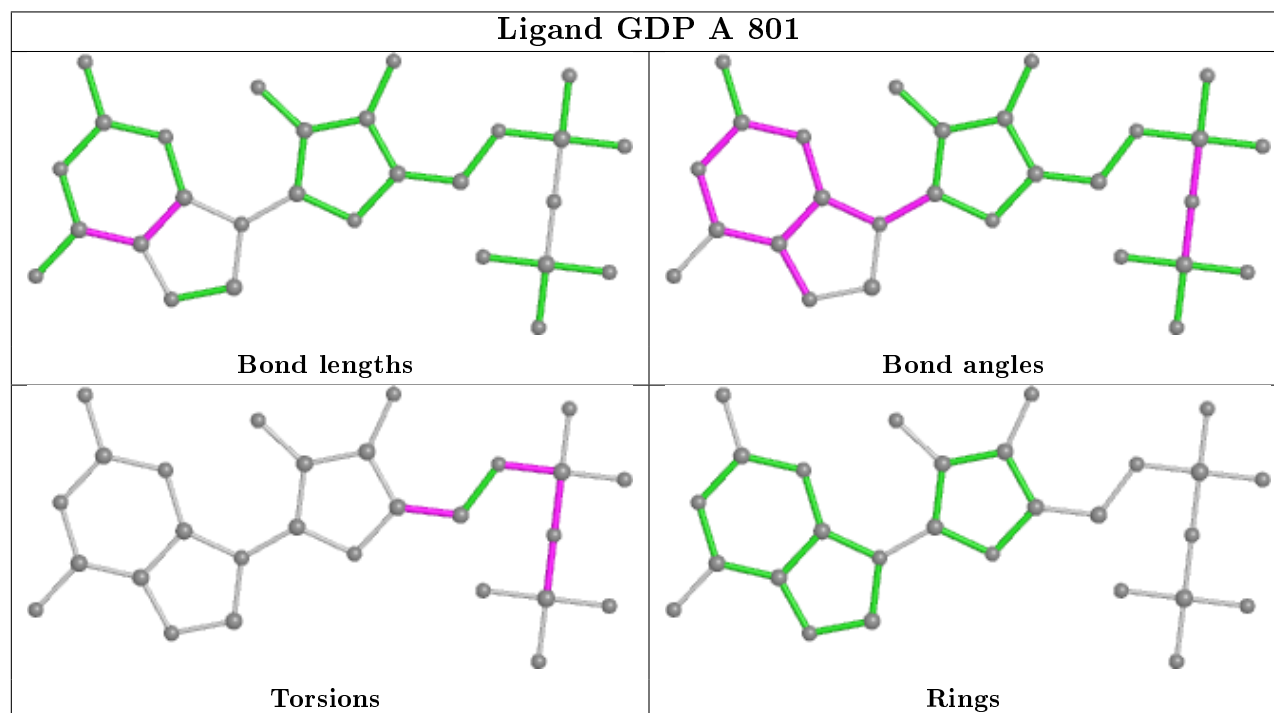
Mol	Chain	Res	Type	Atoms
3	A	801	GDP	PA-O3A-PB-O2B
3	A	801	GDP	C5'-O5'-PA-O1A
3	C	801	GDP	O4'-C4'-C5'-O5'
3	A	801	GDP	O4'-C4'-C5'-O5'
3	A	801	GDP	C3'-C4'-C5'-O5'
3	A	801	GDP	PB-O3A-PA-O2A
3	C	801	GDP	PA-O3A-PB-O1B
3	A	801	GDP	PA-O3A-PB-O3B
3	C	801	GDP	PA-O3A-PB-O2B
3	C	801	GDP	PA-O3A-PB-O3B
3	A	801	GDP	C5'-O5'-PA-O3A
3	A	801	GDP	PB-O3A-PA-O1A

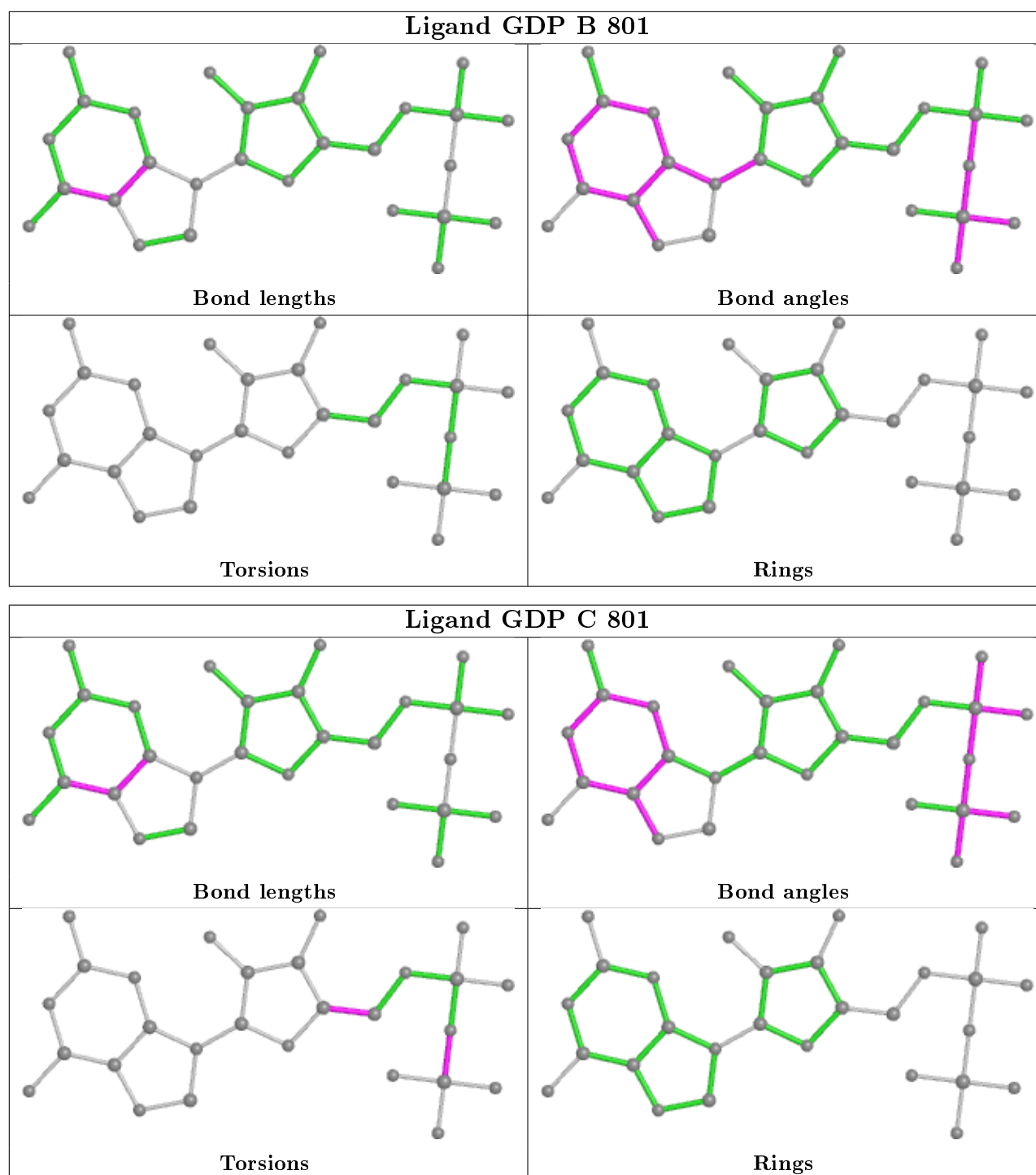
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	GDP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	390/421 (92%)	0.34	4 (1%) 82 72	48, 81, 120, 149	0
2	B	387/421 (91%)	0.40	5 (1%) 77 65	54, 84, 128, 175	0
2	C	389/421 (92%)	0.28	0 100 100	45, 64, 101, 125	0
All	All	1166/1263 (92%)	0.34	9 (0%) 86 78	45, 75, 119, 175	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	704	GLN	2.9
1	A	305	ALA	2.6
1	A	46	ASP	2.6
1	A	139	ASN	2.5
2	B	358	VAL	2.4
2	B	45	LEU	2.4
1	A	154	ALA	2.2
2	B	36	VAL	2.0
2	B	41	LYS	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

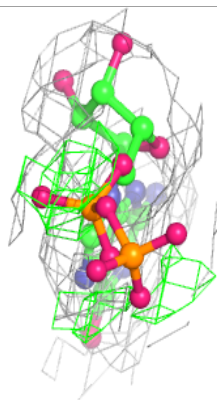
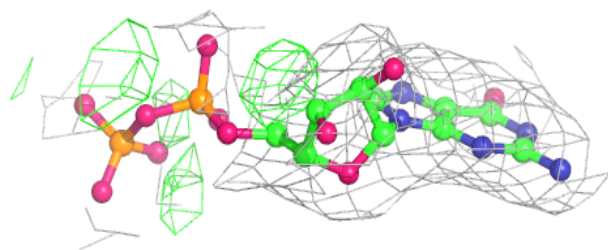
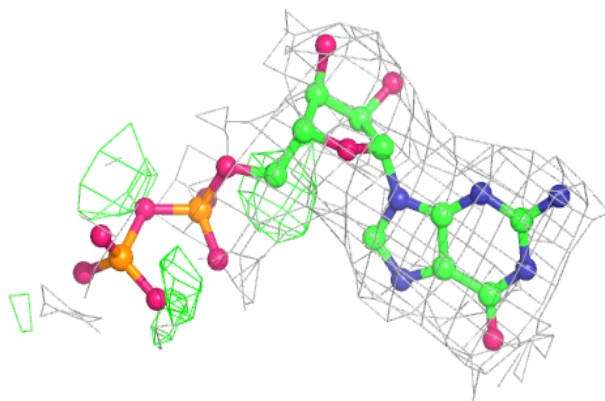
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	K	B	803	1/1	0.85	0.15	78,78,78,78	0
4	BEF	B	802	4/4	0.88	0.43	75,76,99,107	0
6	MG	B	804	1/1	0.90	0.26	46,46,46,46	0
4	BEF	C	802	4/4	0.95	0.39	48,57,68,70	0
5	K	C	803	1/1	0.95	0.19	65,65,65,65	0
4	BEF	A	802	4/4	0.96	0.28	53,59,64,69	0
3	GDP	A	801	28/28	0.97	0.22	45,59,78,89	0
3	GDP	C	801	28/28	0.97	0.24	44,55,64,77	0
5	K	A	803	1/1	0.97	0.14	70,70,70,70	0
6	MG	A	804	1/1	0.97	0.23	52,52,52,52	0
3	GDP	B	801	28/28	0.98	0.21	57,69,78,87	0
6	MG	C	804	1/1	0.98	0.28	37,37,37,37	0

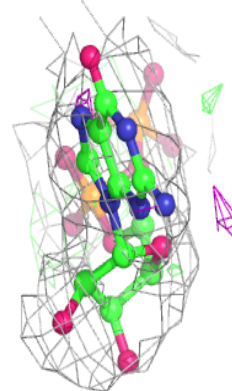
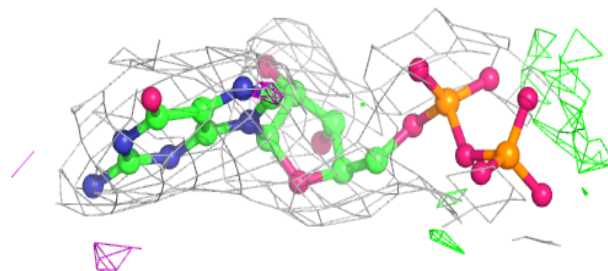
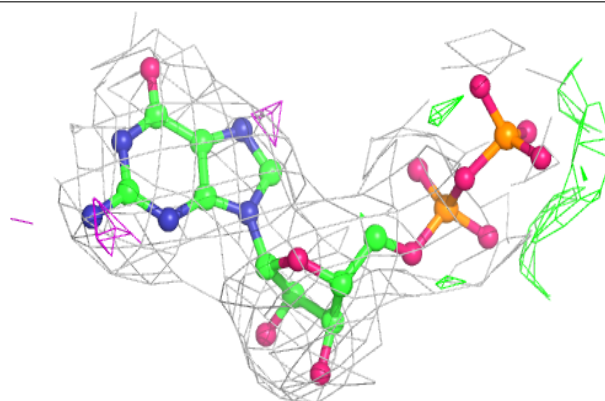
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

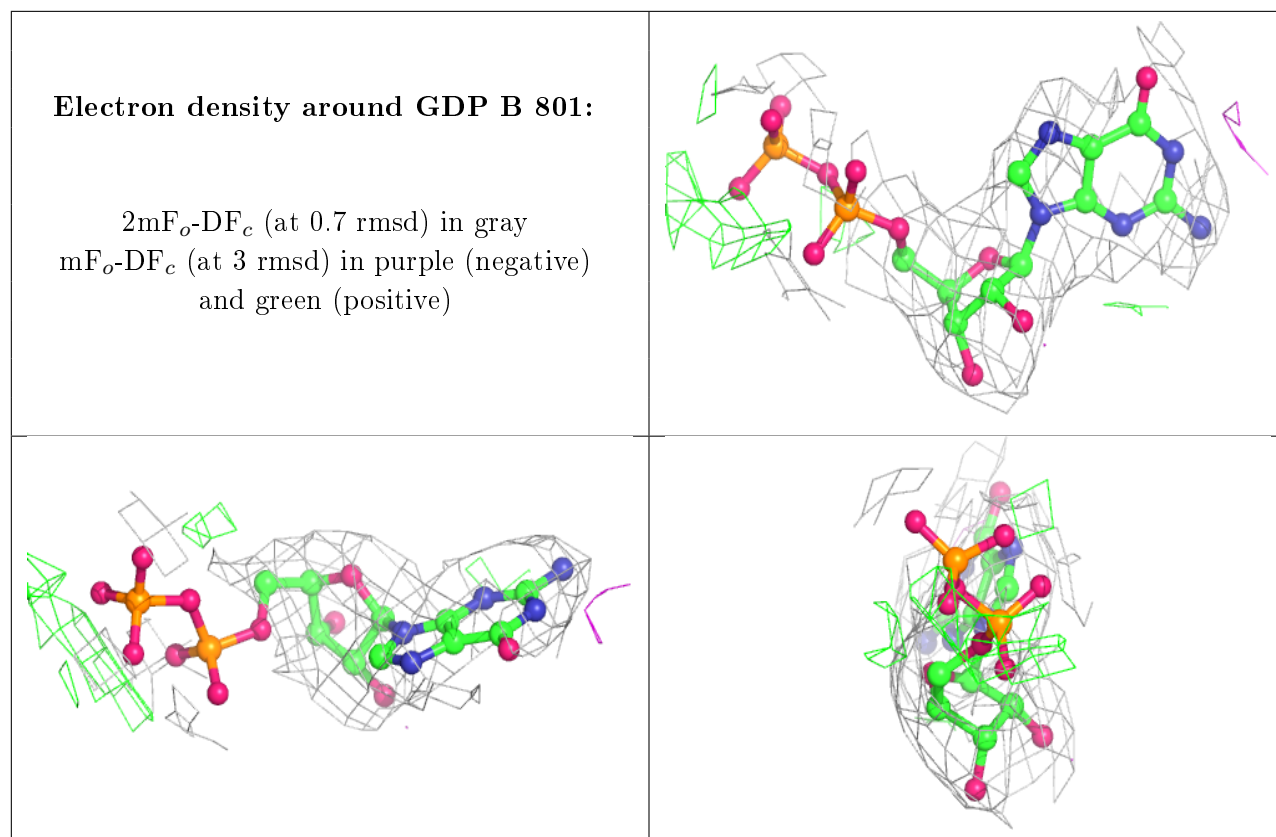
Electron density around GDP A 801:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around GDP C 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 [i](#)

There are no such residues in this entry.