Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:40 PM GMT

PDB ID	:	4U0M
Title	:	Structure of the Vibrio cholerae di-nucleotide cyclase (DncV) mutant D193N in complex with ATP, GTP and 5MTHFGLU2
Authors	:	Zhu, D.; Xiang, Y.
Deposited on	:	2014-07-12
Resolution	:	2.30 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

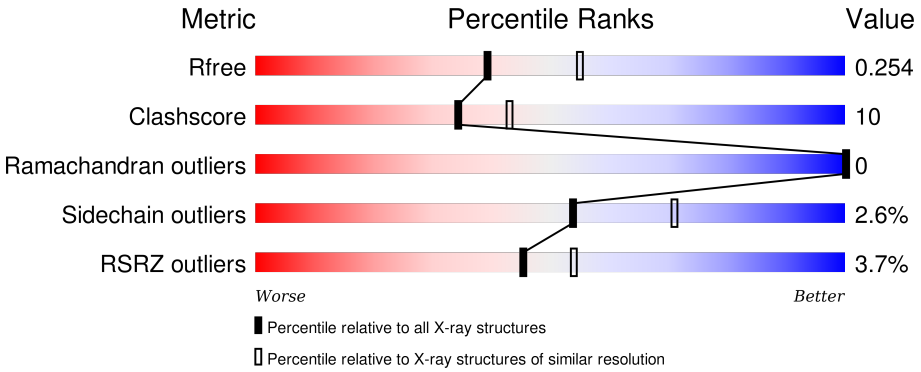
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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 <=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	427	% 71% 18% • 9%
1	B	427	6% 69% 20% • 9%

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
3	ATP	A	502	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6834 atoms, of which 29 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.

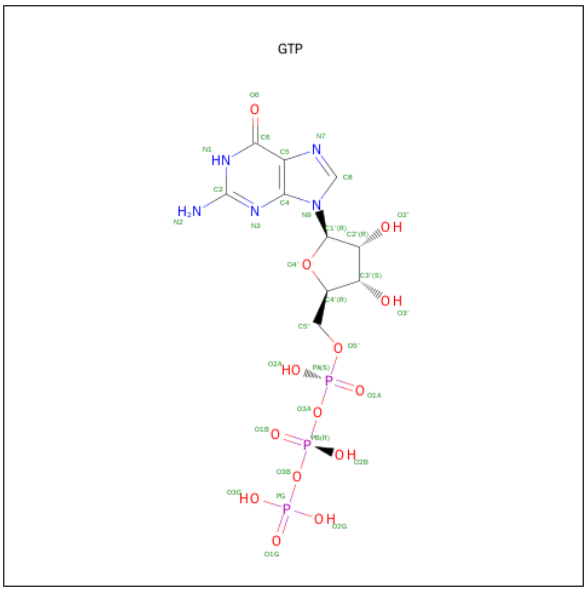
- Molecule 1 is a protein called Cyclic AMP-GMP synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	387	Total	C	N	O	S	0	1	0
			3114	1966	541	591	16			
1	B	388	Total	C	N	O	S	0	0	0
			3113	1965	539	593	16			

There are 18 discrepancies between the modelled and reference sequences:

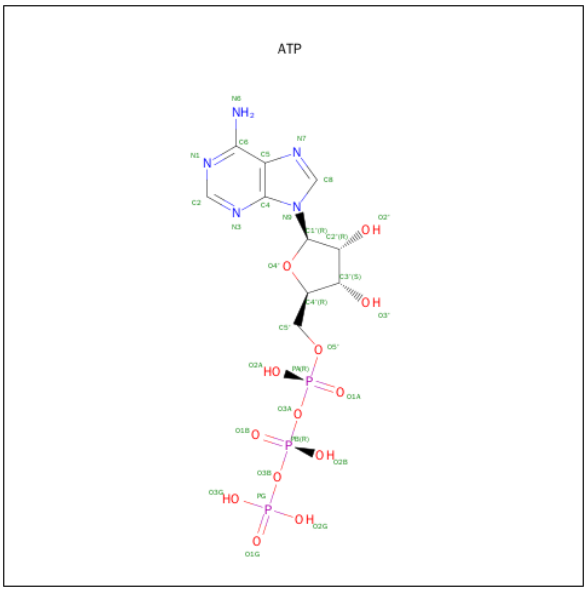
Chain	Residue	Modelled	Actual	Comment	Reference
A	193	ASN	ASP	engineered mutation	UNP Q9KVG7
A	420	LEU	-	expression tag	UNP Q9KVG7
A	421	GLU	-	expression tag	UNP Q9KVG7
A	422	HIS	-	expression tag	UNP Q9KVG7
A	423	HIS	-	expression tag	UNP Q9KVG7
A	424	HIS	-	expression tag	UNP Q9KVG7
A	425	HIS	-	expression tag	UNP Q9KVG7
A	426	HIS	-	expression tag	UNP Q9KVG7
A	427	HIS	-	expression tag	UNP Q9KVG7
B	193	ASN	ASP	engineered mutation	UNP Q9KVG7
B	420	LEU	-	expression tag	UNP Q9KVG7
B	421	GLU	-	expression tag	UNP Q9KVG7
B	422	HIS	-	expression tag	UNP Q9KVG7
B	423	HIS	-	expression tag	UNP Q9KVG7
B	424	HIS	-	expression tag	UNP Q9KVG7
B	425	HIS	-	expression tag	UNP Q9KVG7
B	426	HIS	-	expression tag	UNP Q9KVG7
B	427	HIS	-	expression tag	UNP Q9KVG7

- Molecule 2 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	B	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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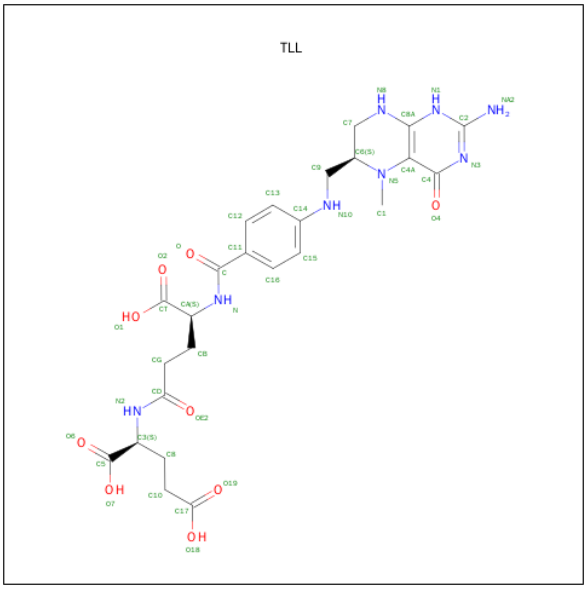
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	1
			62	20	10	26	6		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is N-[4-({[(6S)-2-amino-5-methyl-4-oxo-1,4,5,6,7,8-hexahydropteridin-6-yl]methyl}amino)benzoyl]-L-gamma-glutamyl-L-glutamic acid (three-letter code: TLL) (formula: $C_{25}H_{32}N_8O_9$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	0	0
			71	25	29	8	9		

- Molecule 6 is water.

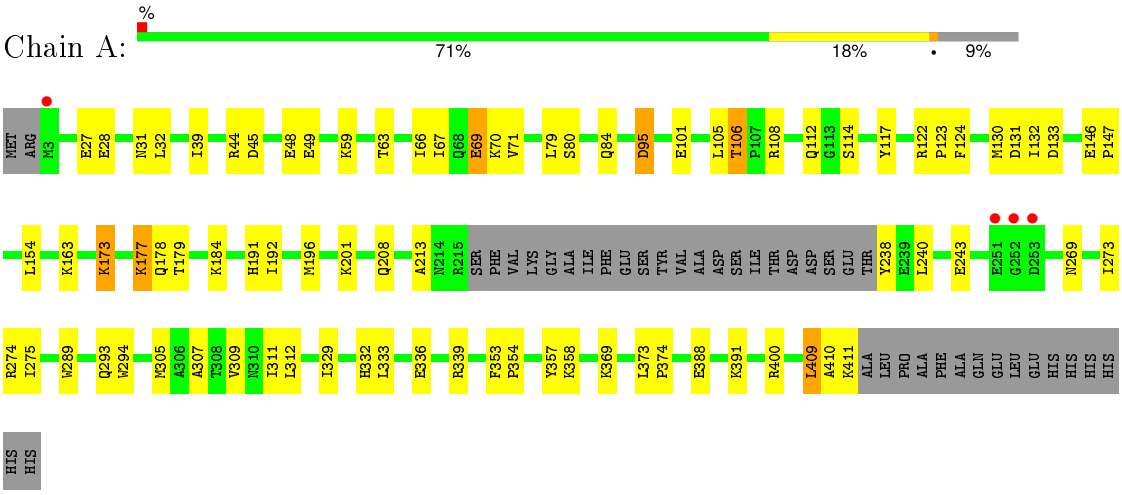
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	191	Total	O	0	0
			191	191		
6	B	186	Total	O	0	0
			186	186		

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.

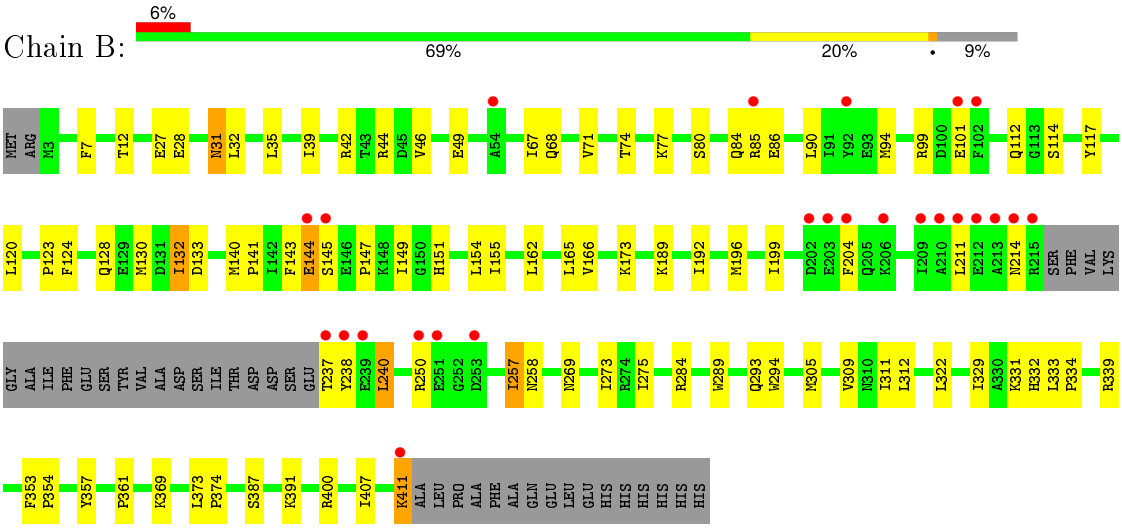
- Molecule 1: Cyclic AMP-GMP synthase

Chain A:



- Molecule 1: Cyclic AMP-GMP synthase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	69.90Å 59.86Å 104.19Å 90.00° 95.55° 90.00°	Depositor
Resolution (Å)	42.57 – 2.30 45.38 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.1 (42.57-2.30) 95.0 (45.38-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.68 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.199 , 0.253 0.203 , 0.254	Depositor DCC
R_{free} test set	1916 reflections (5.51%)	DCC
Wilson B-factor (Å^2)	28.8	Xtriage
Anisotropy	0.666	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 43.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 38298 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6834	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.38% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GTP, MG, ATP, TLL

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	0.20	0/3178	0.35	0/4281
1	B	0.21	0/3174	0.36	0/4277
All	All	0.20	0/6352	0.36	0/8558

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	3114	0	3113	59	0
1	B	3113	0	3107	67	0
2	A	32	0	12	0	0
2	B	32	0	12	1	0
3	A	31	0	12	1	0
3	B	62	0	24	4	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	42	29	29	3	0
6	A	191	0	0	3	0
6	B	186	0	0	7	0
All	All	6805	29	6309	127	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 10.

All (127) 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:A:39:ILE:HD12	1:A:192:ILE:HD13	1.34	1.07
1:A:178:GLN:HG3	1:A:179:THR:HG23	1.59	0.83
1:B:132:ILE:HD13	1:B:132:ILE:H	1.55	0.72
1:B:140:MET:HB2	1:B:141:PRO:HD2	1.74	0.69
1:A:240:LEU:H	5:A:504:TLL:HN1	1.41	0.69
1:B:311:ILE:HD12	1:B:332:HIS:HB3	1.75	0.68
1:B:411:LYS:HB3	1:B:411:LYS:HZ2	1.57	0.68
1:A:32:LEU:HD22	1:A:132:ILE:HD11	1.76	0.68
1:A:294:TRP:CZ2	1:A:369:LYS:HG3	2.29	0.67
1:B:211:LEU:HD22	1:B:238:TYR:CE1	2.30	0.67
1:A:44[B]:ARG:HH22	5:A:504:TLL:CT	2.09	0.66
1:B:77:LYS:NZ	6:B:601:HOH:O	2.29	0.65
1:B:39:ILE:HG13	1:B:192:ILE:HD13	1.79	0.63
1:B:99:ARG:NH2	6:B:703:HOH:O	2.32	0.61
1:A:177:LYS:HE3	1:A:177:LYS:HA	1.81	0.61
1:B:257:ILE:HD13	1:B:258:ASN:N	2.15	0.60
1:B:331:LYS:HE3	1:B:332:HIS:CE1	2.37	0.59
1:B:294:TRP:CZ2	1:B:369:LYS:HD2	2.38	0.59
1:B:112:GLN:O	1:B:133:ASP:HB2	2.04	0.58
1:B:123:PRO:HD3	1:B:130:MET:HG3	1.86	0.58
1:B:149:ILE:HD12	1:B:149:ILE:H	1.69	0.57
1:A:213:ALA:HA	1:B:339:ARG:HD3	1.85	0.57
1:B:411:LYS:H	1:B:411:LYS:HZ3	1.53	0.57
1:A:173:LYS:HG2	1:A:184:LYS:HB3	1.88	0.56
1:B:143:PHE:CD1	1:B:147:PRO:HB3	2.41	0.56
3:B:502[A]:ATP:N6	6:B:739:HOH:O	2.40	0.55
1:B:411:LYS:H	1:B:411:LYS:NZ	2.05	0.55
1:A:63:THR:OG1	1:A:66:ILE:HG12	2.06	0.54
1:B:211:LEU:HD12	1:B:214:ASN:ND2	2.23	0.53
1:B:101:GLU:HB3	1:B:149:ILE:HD11	1.91	0.53
1:B:149:ILE:N	1:B:149:ILE:HD12	2.24	0.52
3:B:502[A]:ATP:N3	6:B:776:HOH:O	2.34	0.52
1:B:27:GLU:O	1:B:31:ASN:HB2	2.10	0.52
1:B:373:LEU:N	1:B:374:PRO:HD2	2.25	0.52
1:B:204:PHE:HE1	1:B:237:THR:HA	1.75	0.52
1:B:80:SER:O	1:B:84:GLN:HG3	2.10	0.52
1:A:133:ASP:OD1	3:A:502:ATP:O3'	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:LEU:HB3	1:A:132:ILE:CD1	2.41	0.51
1:B:269:ASN:O	1:B:273:ILE:HG12	2.11	0.51
1:A:373:LEU:N	1:A:374:PRO:HD2	2.25	0.51
1:A:79:LEU:HD23	1:A:163:LYS:HD2	1.92	0.51
1:B:144:GLU:O	1:B:145:SER:HB3	2.11	0.50
1:A:112:GLN:O	1:A:133:ASP:HB2	2.12	0.50
1:B:250:ARG:NH2	6:B:733:HOH:O	2.44	0.49
1:A:131:ASP:HB3	1:A:191:HIS:CE1	2.47	0.49
1:B:132:ILE:HG12	1:B:192:ILE:HG13	1.93	0.49
1:A:124:PHE:HB2	1:A:400:ARG:NH2	2.26	0.49
1:B:35:LEU:O	1:B:39:ILE:HG12	2.12	0.49
1:A:274:ARG:NH2	6:A:665:HOH:O	2.39	0.49
1:A:311:ILE:HD12	1:A:332:HIS:CB	2.42	0.49
1:B:68:GLN:NE2	1:B:85:ARG:HG2	2.28	0.48
1:A:63:THR:O	1:A:67:ILE:HG12	2.14	0.48
1:B:154:LEU:HB3	1:B:196:MET:SD	2.53	0.48
1:A:28:GLU:OE2	1:A:122:ARG:NH1	2.42	0.48
1:A:80:SER:O	1:A:84:GLN:HG3	2.13	0.48
1:B:329:ILE:O	1:B:333:LEU:HG	2.14	0.48
1:B:42:ARG:HG2	1:B:165:LEU:HG	1.96	0.47
1:B:67:ILE:O	1:B:71:VAL:HG23	2.14	0.47
1:B:7:PHE:CD1	1:B:407:ILE:HD12	2.49	0.47
1:A:409:LEU:HD13	1:A:410:ALA:N	2.30	0.47
1:A:388:GLU:HA	1:A:391:LYS:HE3	1.96	0.47
1:A:39:ILE:CD1	1:A:192:ILE:HG21	2.45	0.47
1:A:275:ILE:HD13	1:A:312:LEU:HB2	1.96	0.47
1:B:311:ILE:CD1	1:B:332:HIS:HB3	2.45	0.47
1:A:311:ILE:HD12	1:A:332:HIS:HB3	1.95	0.47
1:A:357:TYR:CE2	1:A:358:LYS:HG3	2.49	0.47
1:A:101:GLU:OE1	1:A:201:LYS:NZ	2.47	0.47
1:A:32:LEU:HB3	1:A:132:ILE:HD11	1.97	0.46
1:B:123:PRO:HD3	1:B:130:MET:CG	2.44	0.46
1:B:331:LYS:HE3	1:B:332:HIS:HE1	1.80	0.46
1:B:12:THR:CG2	1:B:322:LEU:HD12	2.45	0.46
1:A:123:PRO:HD3	1:A:130:MET:CG	2.45	0.46
1:A:95:ASP:OD1	1:A:95:ASP:N	2.46	0.46
1:B:42:ARG:O	1:B:46:VAL:HG23	2.15	0.46
1:A:388:GLU:HG3	1:A:391:LYS:NZ	2.31	0.46
1:A:329:ILE:O	1:A:333:LEU:HG	2.16	0.46
1:A:289:TRP:O	1:A:293:GLN:HG2	2.16	0.46
1:A:45:ASP:O	1:A:49:GLU:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:GLU:HG3	1:B:361:PRO:HG2	1.98	0.46
2:B:501:GTP:H5'	3:B:502[B]:ATP:O2'	2.14	0.45
1:A:339:ARG:HG3	6:A:610:HOH:O	2.16	0.45
1:B:387:SER:O	1:B:391:LYS:HG3	2.16	0.45
1:A:311:ILE:HD11	1:A:336:GLU:CG	2.46	0.45
1:B:28:GLU:O	1:B:32:LEU:HG	2.16	0.45
1:A:32:LEU:CD2	1:A:132:ILE:HD11	2.45	0.45
1:A:357:TYR:CD2	1:A:358:LYS:HG3	2.51	0.45
1:A:131:ASP:HB3	1:A:191:HIS:NE2	2.32	0.45
1:A:44[B]:ARG:NH2	5:A:504:TLL:O2	2.50	0.45
1:A:67:ILE:O	1:A:71:VAL:HG23	2.16	0.45
1:B:237:THR:HG22	1:B:240:LEU:HD11	1.98	0.45
1:B:143:PHE:CG	1:B:147:PRO:HB3	2.52	0.45
1:A:269:ASN:O	1:A:273:ILE:HG12	2.17	0.45
1:A:69:GLU:HG3	1:A:70:LYS:N	2.32	0.45
1:B:132:ILE:HD13	1:B:132:ILE:N	2.28	0.44
1:B:353:PHE:HA	1:B:354:PRO:HD3	1.84	0.44
1:B:162:LEU:O	1:B:166:VAL:HG23	2.17	0.44
1:B:289:TRP:O	1:B:293:GLN:HG2	2.16	0.44
3:B:502[B]:ATP:N6	6:B:739:HOH:O	2.41	0.44
1:B:151:HIS:O	1:B:155:ILE:HG12	2.18	0.44
1:A:154:LEU:HB3	1:A:196:MET:SD	2.58	0.44
1:B:44:ARG:NH1	6:B:693:HOH:O	2.31	0.44
1:A:39:ILE:HD11	1:A:192:ILE:HG21	1.98	0.44
1:B:305:MET:O	1:B:309:VAL:HG23	2.18	0.43
1:B:124:PHE:HB2	1:B:400:ARG:NH2	2.34	0.43
1:A:146:GLU:CD	1:A:147:PRO:HD2	2.39	0.43
1:B:240:LEU:N	1:B:240:LEU:HD12	2.33	0.43
1:B:275:ILE:HD13	1:B:312:LEU:HB2	2.00	0.43
1:A:305:MET:O	1:A:309:VAL:HG23	2.19	0.43
1:B:120:LEU:O	1:B:284:ARG:NH1	2.48	0.42
1:B:94:MET:O	1:B:99:ARG:NH2	2.53	0.42
1:B:240:LEU:HD12	1:B:240:LEU:H	1.83	0.42
1:B:128:GLN:O	1:B:189:LYS:HE2	2.19	0.42
1:A:388:GLU:HA	1:A:391:LYS:CE	2.50	0.42
1:B:199:ILE:HB	1:B:240:LEU:HD22	2.02	0.42
1:B:32:LEU:HD22	1:B:132:ILE:HD12	2.02	0.42
1:B:49:GLU:OE1	1:B:74:THR:HB	2.18	0.42
1:A:131:ASP:HA	1:A:191:HIS:O	2.19	0.41
1:A:339:ARG:NH1	6:A:734:HOH:O	2.46	0.41
1:A:27:GLU:O	1:A:31:ASN:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:GLN:HG2	1:B:357:TYR:HB3	2.01	0.41
1:A:114:SER:HA	1:A:117:TYR:CE1	2.55	0.41
1:A:106:THR:OG1	1:A:108:ARG:HD3	2.21	0.41
1:A:307:ALA:O	1:A:311:ILE:HG12	2.21	0.41
1:A:353:PHE:HA	1:A:354:PRO:HD3	1.82	0.41
1:B:114:SER:HA	1:B:117:TYR:CE1	2.56	0.41
1:B:333:LEU:HB2	1:B:334:PRO:HD3	2.03	0.40
1:B:86:GLU:O	1:B:90:LEU:HG	2.20	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	384/427 (90%)	375 (98%)	9 (2%)	0	100	100
1	B	384/427 (90%)	371 (97%)	13 (3%)	0	100	100
All	All	768/854 (90%)	746 (97%)	22 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	342/375 (91%)	331 (97%)	11 (3%)	46	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	342/375 (91%)	335 (98%)	7 (2%)	63 79
All	All	684/750 (91%)	666 (97%)	18 (3%)	54 71

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	LYS
1	A	69	GLU
1	A	95	ASP
1	A	105	LEU
1	A	106	THR
1	A	173	LYS
1	A	177	LYS
1	A	238	TYR
1	A	243	GLU
1	A	409	LEU
1	A	411	LYS
1	B	31	ASN
1	B	132	ILE
1	B	144	GLU
1	B	173	LYS
1	B	240	LEU
1	B	257	ILE
1	B	411	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	HIS
1	B	116	GLN
1	B	125	GLN
1	B	208	GLN

5.3.3 RNA

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 8 ligands modelled in this entry, 2 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	$\#\|Z\| > 2$
2	GTP	A	501	4	25,34,34	1.14	2 (8%)	34,54,54	1.93	9 (26%)
3	ATP	A	502	-	24,33,33	0.97	1 (4%)	31,52,52	1.99	5 (16%)
5	TLL	A	504	-	30,44,44	4.23	13 (43%)	30,61,61	1.69	5 (16%)
2	GTP	B	501	4	25,34,34	1.15	2 (8%)	34,54,54	2.02	8 (23%)
3	ATP	B	502[A]	-	24,33,33	0.96	1 (4%)	31,52,52	1.91	5 (16%)
3	ATP	B	502[B]	-	24,33,33	0.96	1 (4%)	31,52,52	1.95	5 (16%)

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	GTP	A	501	4	-	0/18/38/38	0/3/3/3
3	ATP	A	502	-	-	0/18/38/38	0/3/3/3
5	TLL	A	504	-	-	0/25/48/48	0/3/3/3
2	GTP	B	501	4	-	0/18/38/38	0/3/3/3
3	ATP	B	502[A]	-	-	0/18/38/38	0/3/3/3
3	ATP	B	502[B]	-	-	0/18/38/38	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	504	TLL	C6-N5	-3.97	1.43	1.47
5	A	504	TLL	C3-N2	-2.68	1.42	1.46
5	A	504	TLL	C7-N8	-2.29	1.43	1.46
5	A	504	TLL	CA-N	-2.09	1.43	1.46
2	B	501	GTP	C5-C4	3.09	1.47	1.40
2	A	501	GTP	C5-C4	3.11	1.47	1.40
3	B	502[A]	ATP	C5-C4	3.14	1.47	1.40
3	A	502	ATP	C5-C4	3.16	1.47	1.40
3	B	502[B]	ATP	C5-C4	3.18	1.47	1.40
2	A	501	GTP	C6-C5	3.69	1.48	1.41
2	B	501	GTP	C6-C5	3.69	1.48	1.41
5	A	504	TLL	C-N	4.98	1.45	1.34
5	A	504	TLL	CD-N2	5.30	1.44	1.34
5	A	504	TLL	C8A-N8	5.31	1.42	1.35
5	A	504	TLL	O4-C4	6.61	1.40	1.24
5	A	504	TLL	C2-NA2	7.84	1.43	1.32
5	A	504	TLL	C16-C11	7.89	1.52	1.39
5	A	504	TLL	C15-C14	8.23	1.52	1.39
5	A	504	TLL	C12-C13	8.35	1.53	1.38
5	A	504	TLL	C4-N3	9.82	1.51	1.33

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	502[A]	ATP	N3-C2-N1	-6.78	123.70	128.89
3	B	502[B]	ATP	N3-C2-N1	-6.76	123.72	128.89
3	A	502	ATP	N3-C2-N1	-6.67	123.78	128.89
2	B	501	GTP	PA-O3A-PB	-5.55	117.13	132.73
3	A	502	ATP	PA-O3A-PB	-4.34	120.53	132.73
2	A	501	GTP	PA-O3A-PB	-4.28	120.72	132.73
2	A	501	GTP	C5-C6-N1	-4.10	117.98	123.59
2	B	501	GTP	C5-C6-N1	-4.09	117.99	123.59
3	B	502[B]	ATP	C2'-C1'-N9	-3.95	108.26	114.29
5	A	504	TLL	C4A-C4-N3	-3.65	117.85	123.46
3	B	502[A]	ATP	PA-O3A-PB	-3.62	122.57	132.73
3	A	502	ATP	C2'-C1'-N9	-3.55	108.86	114.29
2	B	501	GTP	C2'-C1'-N9	-3.55	108.87	114.29
3	A	502	ATP	PB-O3B-PG	-3.53	120.81	132.67
3	B	502[B]	ATP	PA-O3A-PB	-3.46	123.02	132.73
5	A	504	TLL	N1-C2-N3	-3.40	117.24	121.79
3	B	502[B]	ATP	PB-O3B-PG	-3.39	121.30	132.67
2	A	501	GTP	C2'-C1'-N9	-3.28	109.28	114.29
2	B	501	GTP	C4-C5-N7	-3.24	106.50	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	GTP	PB-O3B-PG	-3.17	122.03	132.67
2	A	501	GTP	C4-C5-N7	-3.12	106.61	109.48
2	A	501	GTP	C6-C5-C4	-3.08	117.21	120.90
3	B	502[A]	ATP	PB-O3B-PG	-3.06	122.40	132.67
2	B	501	GTP	C6-C5-C4	-3.06	117.24	120.90
3	B	502[A]	ATP	C4-C5-N7	-3.05	106.68	109.48
2	A	501	GTP	N3-C2-N1	-3.02	122.84	127.44
3	B	502[B]	ATP	C4-C5-N7	-3.02	106.70	109.48
2	B	501	GTP	N3-C2-N1	-3.01	122.86	127.44
3	A	502	ATP	C4-C5-N7	-3.00	106.72	109.48
3	B	502[A]	ATP	C2'-C1'-N9	-2.94	109.81	114.29
2	B	501	GTP	PB-O3B-PG	-2.38	124.67	132.67
2	A	501	GTP	O3G-PG-O2G	2.05	115.20	107.38
5	A	504	TLL	CG-CD-N2	2.71	120.26	115.83
5	A	504	TLL	NA2-C2-N1	3.41	121.52	117.80
5	A	504	TLL	C4-C4A-C8A	4.46	117.98	114.43
2	A	501	GTP	C6-N1-C2	4.60	122.32	115.94
2	B	501	GTP	C6-N1-C2	4.60	122.33	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	ATP	1	0
5	A	504	TLL	3	0
2	B	501	GTP	1	0
3	B	502[A]	ATP	2	0
3	B	502[B]	ATP	2	0

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	387/427 (90%)	-0.08	4 (1%) 84 88	15, 29, 62, 88	0
1	B	388/427 (90%)	0.27	25 (6%) 23 31	15, 33, 85, 104	0
All	All	775/854 (90%)	0.10	29 (3%) 45 54	15, 31, 78, 104	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	212	GLU	7.3
1	B	215	ARG	7.2
1	B	213	ALA	7.1
1	B	211	LEU	6.2
1	B	238	TYR	6.0
1	B	210	ALA	5.3
1	A	252	GLY	5.2
1	B	209	ILE	4.7
1	B	411	LYS	4.6
1	B	237	THR	4.2
1	B	239	GLU	3.2
1	B	251	GLU	3.2
1	B	92	TYR	3.1
1	A	3	MET	3.0
1	B	204	PHE	2.8
1	B	250	ARG	2.8
1	B	144	GLU	2.7
1	B	145	SER	2.7
1	B	214	ASN	2.6
1	A	253	ASP	2.5
1	B	253	ASP	2.5
1	B	202	ASP	2.4
1	B	206	LYS	2.4
1	B	101	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	102	PHE	2.4
1	A	251	GLU	2.1
1	B	54	ALA	2.1
1	B	203	GLU	2.1
1	B	85	ARG	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, 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	LLDF	B-factors(Å^2)	Q<0.9
3	ATP	A	502	31/31	0.62	0.28	5.15	64,96,146,148	0
3	ATP	B	502[A]	31/31	0.87	0.17	1.65	43,49,59,61	31
3	ATP	B	502[B]	31/31	0.87	0.17	1.57	27,49,60,63	31
5	TLL	A	504	42/42	0.91	0.19	1.42	17,32,106,118	0
2	GTP	B	501	32/32	0.96	0.13	0.21	16,27,37,50	0
2	GTP	A	501	32/32	0.97	0.11	-0.24	14,22,32,45	0
4	MG	B	503	1/1	0.86	0.12	-	18,18,18,18	0
4	MG	A	503	1/1	0.89	0.09	-	14,14,14,14	0

6.5 Other polymers (i)

There are no such residues in this entry.