



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:21 AM GMT

PDB ID : 3EC1  
Title : Structure of YqeH GTPase from Geobacillus stearothermophilus (an AtNOS1 / AtNOA1 ortholog)  
Authors : Sudhamsu, J.; Crane, B.R.  
Deposited on : 2008-08-28  
Resolution : 2.36 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

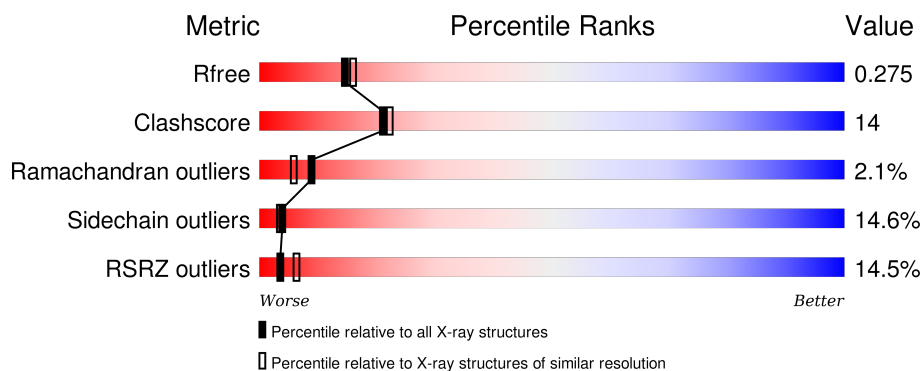
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.36 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	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	369	<div> <div>13%</div> <div> <div></div> <div>55%</div> <div>23%</div> <div>6%</div> <div>•</div> <div>16%</div> </div> </div>
1	B	369	<div> <div>12%</div> <div> <div></div> <div>58%</div> <div>21%</div> <div>5%</div> <div>•</div> <div>16%</div> </div> </div>

## 2 Entry composition [i](#)

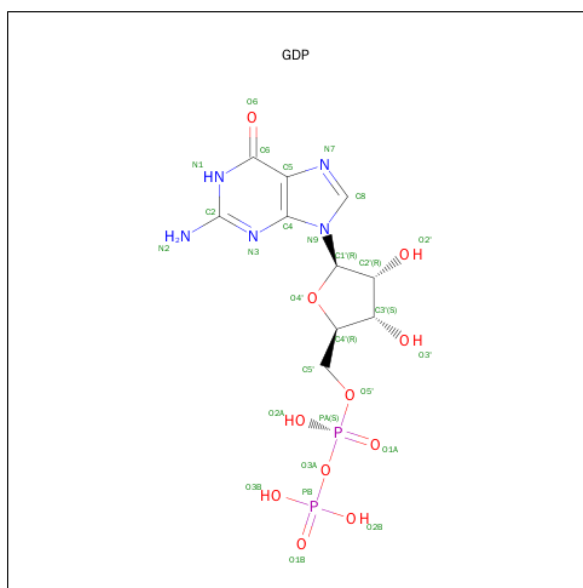
There are 3 unique types of molecules in this entry. The entry contains 5245 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 YqeH GTPase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	311	Total	C	N	O	S	0	0	0
			2427	1554	423	437	13			
1	B	311	Total	C	N	O	S	0	0	0
			2427	1554	423	437	13			

- 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
2	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
2	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

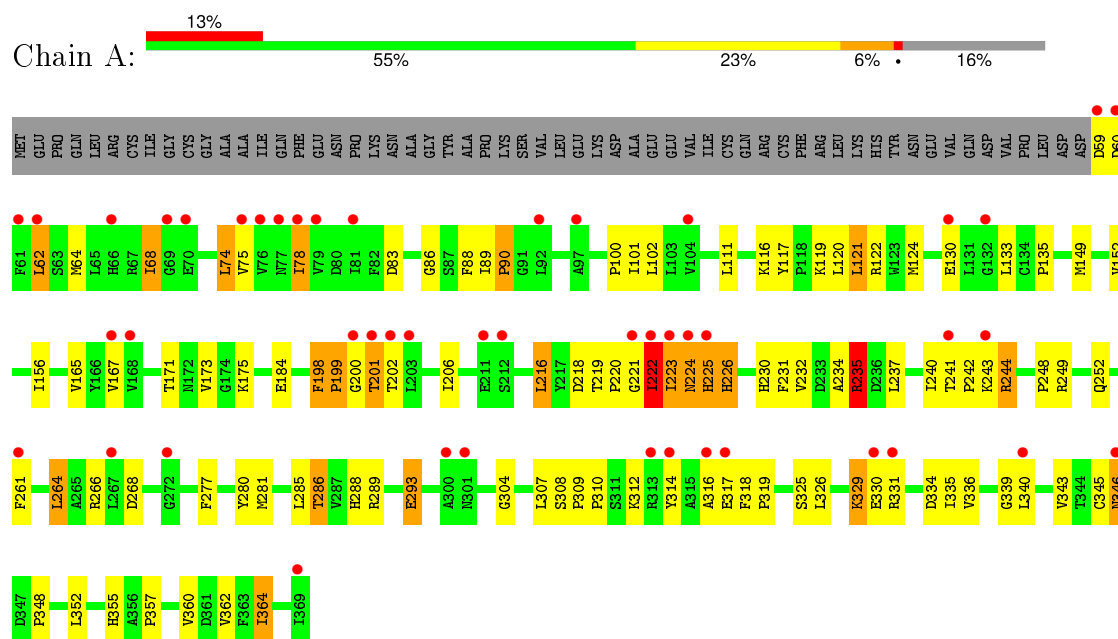
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	167	Total 167	O 167	0	0
3	B	168	Total 168	O 168	0	0

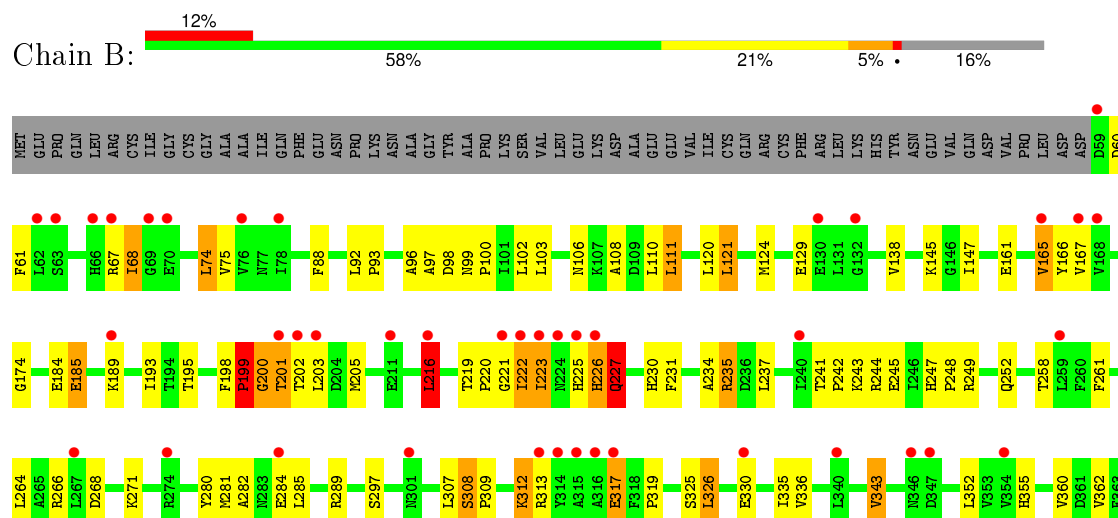
### 3 Residue-property plots

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: YqeH GTPase



#### • Molecule 1: YqeH GTPase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	47.62Å 81.10Å 108.17Å 90.00° 91.50° 90.00°	Depositor
Resolution (Å)	30.00 – 2.36 29.82 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.4 (30.00-2.36) 94.5 (29.82-2.35)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.05 (at 2.36Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.254 , 0.287 0.235 , 0.275	Depositor DCC
$R_{free}$ test set	1613 reflections (4.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	41.9	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 67.7	EDS
Estimated twinning fraction	0.032 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 33950 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5245	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.54 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.1287e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

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	0.40	0/2479	0.74	2/3358 (0.1%)
1	B	0.40	0/2479	0.76	3/3358 (0.1%)
All	All	0.40	0/4958	0.75	5/6716 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	216	LEU	CA-CB-CG	7.24	131.95	115.30
1	B	199	PRO	N-CA-C	6.06	127.85	112.10
1	B	200	GLY	N-CA-C	-5.78	98.64	113.10
1	B	216	LEU	CA-CB-CG	5.42	127.78	115.30
1	A	198	PHE	N-CA-C	-5.34	96.58	111.00

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	2427	0	2474	81	0
1	B	2427	0	2474	58	0
2	A	28	0	12	0	0
2	B	28	0	12	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	167	0	0	3	0
3	B	168	0	0	2	0
All	All	5245	0	4972	141	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 14.

All (141) 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:331:ARG:HG2	1:A:348:PRO:HD3	1.49	0.95
1:A:225:HIS:CD2	1:A:226:HIS:H	1.85	0.94
2:B:900:GDP:H5''	2:B:900:GDP:H8	1.34	0.90
2:B:900:GDP:H5''	2:B:900:GDP:C8	2.06	0.89
1:A:225:HIS:HD2	1:A:226:HIS:H	1.30	0.79
1:A:234:ALA:O	1:A:235:ARG:HB2	1.82	0.77
1:A:244:ARG:HG2	1:A:244:ARG:HH11	1.51	0.76
1:A:219:THR:HG23	1:A:220:PRO:HD2	1.72	0.72
1:A:59:ASP:HA	1:A:62:LEU:HD12	1.71	0.71
1:B:121:LEU:HD12	1:B:138:VAL:HG13	1.73	0.71
1:A:88:PHE:CD2	1:A:90:PRO:HD3	2.26	0.70
1:A:224:ASN:ND2	1:A:224:ASN:H	1.88	0.70
1:B:174:GLY:HA2	2:B:900:GDP:O2A	1.91	0.70
1:B:261:PHE:CD2	1:B:281:MET:HE1	2.28	0.69
1:A:222:ILE:O	1:A:223:ILE:HB	1.92	0.68
1:A:64:MET:O	1:A:68:ILE:HG23	1.95	0.67
1:A:89:ILE:HG22	1:A:89:ILE:O	1.94	0.67
1:A:286:THR:HG22	1:A:288:HIS:NE2	2.08	0.67
1:A:225:HIS:CD2	1:A:226:HIS:N	2.61	0.67
1:B:266:ARG:HD2	1:B:355:HIS:CD2	2.33	0.64
1:A:78:ILE:HG12	1:A:173:VAL:HG12	1.82	0.61
1:A:201:THR:HG22	1:A:202:THR:N	2.16	0.61
1:A:293:GLU:HG3	3:A:1068:HOH:O	2.00	0.60
1:A:198:PHE:O	1:A:200:GLY:N	2.35	0.60
1:A:225:HIS:HD2	1:A:226:HIS:ND1	2.00	0.59
1:B:202:THR:HG22	1:B:203:LEU:H	1.67	0.59
1:A:244:ARG:HH11	1:A:244:ARG:CG	2.16	0.59
1:A:308:SER:HA	1:A:309:PRO:C	2.23	0.58
1:A:78:ILE:HG12	1:A:173:VAL:CG1	2.35	0.57
1:B:198:PHE:O	1:B:200:GLY:N	2.30	0.57
1:A:266:ARG:HD2	1:A:355:HIS:CD2	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:ASN:HD22	1:B:174:GLY:HA3	1.68	0.57
1:B:68:ILE:HD11	1:B:75:VAL:CG2	2.35	0.56
1:A:231:PHE:CD1	1:A:319:PRO:HG2	2.41	0.56
1:B:266:ARG:HD3	1:B:268:ASP:OD1	2.06	0.56
1:B:106:ASN:ND2	1:B:174:GLY:HA3	2.21	0.56
1:B:203:LEU:HB3	1:B:220:PRO:HG2	1.89	0.54
1:B:92:LEU:HB3	1:B:93:PRO:HD3	1.88	0.54
1:A:286:THR:CG2	1:A:288:HIS:NE2	2.71	0.54
1:A:364:ILE:HD11	3:A:954:HOH:O	2.09	0.53
1:B:195:THR:HG23	3:B:911:HOH:O	2.08	0.52
1:A:266:ARG:HD3	1:A:268:ASP:OD1	2.09	0.52
1:B:174:GLY:CA	2:B:900:GDP:O2A	2.58	0.52
1:B:110:LEU:HD22	1:B:242:PRO:HB2	1.92	0.52
1:B:234:ALA:O	1:B:235:ARG:HB2	2.10	0.51
1:A:264:LEU:HD12	1:A:318:PHE:CZ	2.46	0.51
1:B:221:GLY:O	1:B:223:ILE:N	2.44	0.51
1:A:225:HIS:CD2	1:A:226:HIS:ND1	2.80	0.50
1:A:314:TYR:C	1:A:316:ALA:H	2.14	0.50
1:B:335:ILE:HD12	1:B:343:VAL:HG22	1.93	0.50
1:B:201:THR:CG2	1:B:202:THR:N	2.75	0.50
1:B:88:PHE:O	1:B:225:HIS:CE1	2.64	0.50
1:B:68:ILE:HD13	1:B:166:TYR:CD1	2.46	0.50
1:A:248:PRO:HG3	1:A:280:TYR:HE1	1.77	0.50
1:A:222:ILE:O	1:A:223:ILE:CB	2.60	0.49
1:B:68:ILE:HD11	1:B:75:VAL:HG22	1.94	0.49
1:A:249:ARG:HD3	3:A:982:HOH:O	2.12	0.49
1:B:261:PHE:HD2	1:B:281:MET:HE1	1.72	0.49
1:B:96:ALA:O	1:B:97:ALA:HB3	2.13	0.49
1:B:201:THR:HG22	1:B:202:THR:N	2.27	0.49
1:B:219:THR:HG23	1:B:220:PRO:HD2	1.94	0.49
1:B:313:ARG:HE	1:B:313:ARG:HA	1.76	0.49
1:B:248:PRO:HG3	1:B:280:TYR:CE1	2.48	0.48
1:A:248:PRO:HG3	1:A:280:TYR:CE1	2.48	0.48
1:B:312:LYS:O	1:B:312:LYS:HG3	2.13	0.48
1:A:225:HIS:CG	1:A:226:HIS:H	2.30	0.48
1:A:86:GLY:HA2	1:A:225:HIS:NE2	2.28	0.48
1:A:223:ILE:HG22	1:A:223:ILE:O	2.14	0.48
1:A:336:VAL:O	1:A:362:VAL:HA	2.14	0.48
1:B:252:GLN:O	1:B:289:ARG:NH2	2.43	0.48
1:B:68:ILE:O	1:B:68:ILE:HD12	2.14	0.48
1:B:313:ARG:HA	1:B:313:ARG:NE	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:GLN:O	1:A:289:ARG:NH2	2.42	0.47
1:A:261:PHE:CD2	1:A:281:MET:HE1	2.49	0.47
1:A:120:LEU:O	1:A:124:MET:HG2	2.15	0.47
1:A:133:LEU:HD22	1:A:135:PRO:HD3	1.97	0.47
1:B:289:ARG:HD2	3:B:2186:HOH:O	2.15	0.47
1:B:308:SER:HA	1:B:309:PRO:C	2.34	0.47
1:B:167:VAL:O	1:B:219:THR:HB	2.15	0.47
1:B:227:GLN:O	1:B:230:HIS:HB3	2.15	0.47
1:B:121:LEU:HD12	1:B:138:VAL:CG1	2.45	0.46
1:A:175:LYS:CE	1:A:221:GLY:HA2	2.45	0.46
1:A:357:PRO:O	1:A:360:VAL:HG13	2.15	0.46
1:A:329:LYS:HB3	1:A:329:LYS:NZ	2.30	0.46
1:A:232:VAL:HG21	1:A:240:ILE:CD1	2.45	0.46
1:A:64:MET:SD	1:A:220:PRO:HD2	2.56	0.45
1:A:89:ILE:O	1:A:90:PRO:C	2.54	0.45
1:B:165:VAL:HG13	1:B:216:LEU:HA	1.97	0.45
1:A:171:THR:HG23	1:A:222:ILE:HA	1.99	0.45
1:B:226:HIS:O	1:B:227:GLN:O	2.34	0.45
1:A:277:PHE:CE1	1:A:345:CYS:SG	3.09	0.45
1:A:86:GLY:C	1:A:225:HIS:CE1	2.90	0.45
1:B:231:PHE:CD1	1:B:319:PRO:HG3	2.51	0.45
1:B:92:LEU:O	1:B:96:ALA:HB3	2.17	0.45
1:A:219:THR:HG23	1:A:220:PRO:CD	2.45	0.44
1:A:304:GLY:HA2	1:A:310:PRO:O	2.17	0.44
1:A:346:ASN:H	1:A:346:ASN:ND2	2.15	0.44
1:A:206:ILE:HB	1:A:218:ASP:HB3	2.00	0.44
1:A:318:PHE:HA	1:A:319:PRO:HD3	1.73	0.44
1:B:241:THR:HA	1:B:242:PRO:HD3	1.87	0.44
1:A:335:ILE:HD12	1:A:343:VAL:HG22	1.99	0.44
1:A:152:VAL:O	1:A:156:ILE:HG13	2.18	0.44
1:A:88:PHE:O	1:A:90:PRO:HD2	2.18	0.43
1:B:336:VAL:O	1:B:362:VAL:HA	2.18	0.43
1:A:74:LEU:HA	1:A:100:PRO:HG2	2.01	0.43
1:B:108:ALA:HA	1:B:111:LEU:HD22	2.00	0.43
1:A:222:ILE:H	1:A:222:ILE:HG12	1.30	0.43
1:B:193:ILE:HD12	1:B:193:ILE:N	2.33	0.43
1:B:325:SER:O	1:B:326:LEU:HD13	2.18	0.43
1:A:334:ASP:O	1:A:364:ILE:HA	2.19	0.43
1:A:232:VAL:HG21	1:A:240:ILE:HD12	2.01	0.43
1:B:222:ILE:O	1:B:223:ILE:HG13	2.19	0.43
1:A:116:LYS:HB2	1:A:119:LYS:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:LEU:HG	1:B:364:ILE:HG22	2.01	0.42
1:A:261:PHE:CD2	1:A:281:MET:CE	3.02	0.42
1:A:244:ARG:CG	1:A:244:ARG:NH1	2.77	0.42
1:B:185:GLU:O	1:B:189:LYS:HG3	2.19	0.42
1:A:225:HIS:CG	1:A:226:HIS:N	2.88	0.42
1:B:120:LEU:O	1:B:124:MET:HG2	2.19	0.42
1:A:281:MET:HE2	1:A:281:MET:HB2	1.45	0.42
1:A:117:TYR:O	1:A:121:LEU:HB2	2.20	0.42
1:A:243:LYS:C	1:A:244:ARG:HG3	2.40	0.41
1:B:258:THR:O	1:B:289:ARG:HA	2.19	0.41
1:B:242:PRO:HG3	1:B:282:ALA:HB2	2.02	0.41
1:B:74:LEU:HA	1:B:100:PRO:HG2	2.02	0.41
1:A:286:THR:CG2	1:A:288:HIS:CE1	3.04	0.41
1:B:248:PRO:HG3	1:B:280:TYR:HE1	1.82	0.41
1:A:241:THR:HA	1:A:242:PRO:HD3	1.87	0.41
1:A:175:LYS:NZ	1:A:221:GLY:HA2	2.35	0.41
1:A:167:VAL:O	1:A:219:THR:HB	2.20	0.41
1:B:145:LYS:HB3	1:B:147:ILE:HD13	2.02	0.41
1:A:89:ILE:CG2	1:A:89:ILE:O	2.63	0.41
1:A:240:ILE:HD11	1:A:264:LEU:HD21	2.01	0.40
1:B:247:HIS:HA	1:B:248:PRO:HD3	1.94	0.40
1:B:111:LEU:O	1:B:245:GLU:HG3	2.21	0.40
1:A:68:ILE:HD11	1:A:75:VAL:CG2	2.51	0.40
1:A:293:GLU:H	1:A:293:GLU:CD	2.25	0.40
1:A:175:LYS:HE3	1:A:221:GLY:HA2	2.04	0.40
1:A:149:MET:O	1:A:152:VAL:HG12	2.20	0.40
1:B:61:PHE:CE2	1:B:222:ILE:O	2.74	0.40
1:A:83:ASP:HB2	1:A:339:GLY:HA2	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	309/369 (84%)	284 (92%)	19 (6%)	6 (2%)	10	7
1	B	309/369 (84%)	286 (93%)	16 (5%)	7 (2%)	8	5
All	All	618/738 (84%)	570 (92%)	35 (6%)	13 (2%)	9	6

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	PRO
1	A	199	PRO
1	A	201	THR
1	A	222	ILE
1	B	199	PRO
1	B	223	ILE
1	B	227	GLN
1	B	235	ARG
1	A	223	ILE
1	A	235	ARG
1	B	222	ILE
1	B	317	GLU
1	B	161	GLU

### 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	264/314 (84%)	226 (86%)	38 (14%)	4	4
1	B	264/314 (84%)	225 (85%)	39 (15%)	4	3
All	All	528/628 (84%)	451 (85%)	77 (15%)	4	3

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	ASP
1	A	62	LEU
1	A	68	ILE

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Mol	Chain	Res	Type
1	A	74	LEU
1	A	78	ILE
1	A	101	ILE
1	A	102	LEU
1	A	111	LEU
1	A	121	LEU
1	A	122	ARG
1	A	130	GLU
1	A	165	VAL
1	A	184	GLU
1	A	199	PRO
1	A	216	LEU
1	A	222	ILE
1	A	224	ASN
1	A	225	HIS
1	A	226	HIS
1	A	230	HIS
1	A	235	ARG
1	A	237	LEU
1	A	244	ARG
1	A	264	LEU
1	A	285	LEU
1	A	286	THR
1	A	293	GLU
1	A	307	LEU
1	A	312	LYS
1	A	317	GLU
1	A	325	SER
1	A	326	LEU
1	A	329	LYS
1	A	330	GLU
1	A	340	LEU
1	A	346	ASN
1	A	352	LEU
1	A	364	ILE
1	B	60	ASP
1	B	67	ARG
1	B	68	ILE
1	B	74	LEU
1	B	98	ASP
1	B	99	ASN
1	B	102	LEU

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Mol	Chain	Res	Type
1	B	103	LEU
1	B	111	LEU
1	B	121	LEU
1	B	129	GLU
1	B	165	VAL
1	B	184	GLU
1	B	185	GLU
1	B	199	PRO
1	B	201	THR
1	B	205	MET
1	B	216	LEU
1	B	226	HIS
1	B	227	GLN
1	B	237	LEU
1	B	243	LYS
1	B	244	ARG
1	B	249	ARG
1	B	264	LEU
1	B	271	LYS
1	B	284	GLU
1	B	285	LEU
1	B	297	SER
1	B	307	LEU
1	B	308	SER
1	B	312	LYS
1	B	317	GLU
1	B	326	LEU
1	B	330	GLU
1	B	343	VAL
1	B	352	LEU
1	B	360	VAL
1	B	364	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	224	ASN
1	A	225	HIS
1	A	230	HIS
1	A	252	GLN
1	A	301	ASN
1	A	346	ASN

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Mol	Chain	Res	Type
1	A	366	GLN
1	B	225	HIS
1	B	301	ASN
1	B	366	GLN

### 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](#)

2 ligands are 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	A	900	-	23,30,30	1.18	2 (8%)	30,47,47	2.89	10 (33%)
2	GDP	B	900	-	23,30,30	1.84	2 (8%)	30,47,47	3.61	17 (56%)

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	A	900	-	-	0/12/32/32	0/3/3/3
2	GDP	B	900	-	-	0/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900	GDP	C8-N7	-2.19	1.30	1.34
2	A	900	GDP	PA-O2A	2.05	1.63	1.54
2	B	900	GDP	PB-O3B	2.34	1.63	1.54
2	B	900	GDP	O4'-C1'	6.68	1.49	1.41

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	900	GDP	C2'-C1'-N9	-8.51	101.29	114.29
2	A	900	GDP	PA-O3A-PB	-7.65	107.02	132.67
2	A	900	GDP	O3A-PA-O5'	-6.97	84.44	102.94
2	A	900	GDP	O5'-PA-O1A	-6.40	84.76	109.62
2	B	900	GDP	PA-O3A-PB	-6.33	111.44	132.67
2	B	900	GDP	O5'-PA-O1A	-6.32	85.10	109.62
2	B	900	GDP	O3A-PA-O5'	-6.09	86.77	102.94
2	B	900	GDP	O2A-PA-O5'	-5.64	80.02	108.46
2	B	900	GDP	O2B-PB-O3A	-5.17	81.62	105.09
2	A	900	GDP	O2A-PA-O5'	-5.01	83.20	108.46
2	B	900	GDP	O3B-PB-O3A	-4.28	85.68	105.09
2	A	900	GDP	C5-C6-N1	-3.82	118.37	123.59
2	A	900	GDP	N3-C2-N1	-3.81	121.64	127.44
2	B	900	GDP	N3-C2-N1	-3.77	121.70	127.44
2	B	900	GDP	C5-C6-N1	-3.62	118.64	123.59
2	B	900	GDP	C4-C5-N7	-2.65	107.04	109.48
2	B	900	GDP	C1'-N9-C4	-2.40	123.33	126.94
2	A	900	GDP	C6-C5-C4	-2.32	118.13	120.90
2	B	900	GDP	C6-C5-C4	-2.22	118.25	120.90
2	B	900	GDP	O3B-PB-O2B	2.59	117.25	107.38
2	A	900	GDP	O2A-PA-O3A	2.87	118.10	105.09
2	A	900	GDP	O4'-C4'-C3'	2.87	110.93	105.15
2	B	900	GDP	C6-N1-C2	2.91	119.97	115.94
2	B	900	GDP	C2'-C3'-C4'	3.11	109.01	102.61
2	A	900	GDP	C6-N1-C2	3.46	120.74	115.94
2	B	900	GDP	O2B-PB-O1B	3.97	123.36	110.58
2	B	900	GDP	O4'-C1'-N9	4.76	118.06	108.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	900	GDP	4	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	311/369 (84%)	0.86	47 (15%) 3 5	17, 42, 79, 95	0
1	B	311/369 (84%)	0.77	43 (13%) 4 8	20, 43, 77, 92	0
All	All	622/738 (84%)	0.82	90 (14%) 3 6	17, 42, 78, 95	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	202	THR	9.4
1	A	317	GLU	8.2
1	B	201	THR	6.8
1	A	221	GLY	6.6
1	B	222	ILE	6.3
1	B	202	THR	5.2
1	A	316	ALA	5.0
1	A	222	ILE	4.9
1	B	67	ARG	4.9
1	B	226	HIS	4.8
1	B	317	GLU	4.5
1	B	346	ASN	4.4
1	A	314	TYR	4.3
1	B	315	ALA	4.0
1	B	316	ALA	4.0
1	A	78	ILE	4.0
1	B	284	GLU	3.8
1	A	76	VAL	3.8
1	B	224	ASN	3.6
1	A	168	VAL	3.5
1	B	66	HIS	3.5
1	B	76	VAL	3.5
1	A	92	LEU	3.5
1	B	211	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	59	ASP	3.4
1	A	301	ASN	3.3
1	A	211	GLU	3.3
1	B	130	GLU	3.3
1	A	201	THR	3.3
1	A	331	ARG	3.3
1	A	203	LEU	3.2
1	A	200	GLY	3.2
1	B	267	LEU	3.2
1	B	167	VAL	3.2
1	B	168	VAL	3.2
1	A	66	HIS	3.1
1	A	267	LEU	3.1
1	B	132	GLY	3.0
1	A	225	HIS	3.0
1	B	314	TYR	3.0
1	A	330	GLU	3.0
1	A	346	ASN	3.0
1	B	313	ARG	2.9
1	B	221	GLY	2.9
1	A	340	LEU	2.9
1	A	313	ARG	2.9
1	A	130	GLU	2.9
1	B	225	HIS	2.8
1	A	104	VAL	2.8
1	B	340	LEU	2.8
1	B	63	SER	2.7
1	B	69	GLY	2.7
1	B	62	LEU	2.7
1	A	272	GLY	2.7
1	B	203	LEU	2.6
1	B	274	ARG	2.6
1	A	60	ASP	2.6
1	B	223	ILE	2.6
1	A	79	VAL	2.5
1	A	70	GLU	2.5
1	B	78	ILE	2.5
1	B	59	ASP	2.5
1	A	212	SER	2.4
1	A	224	ASN	2.4
1	B	165	VAL	2.4
1	A	223	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	240	ILE	2.4
1	A	167	VAL	2.3
1	A	97	ALA	2.3
1	A	61	PHE	2.3
1	B	330	GLU	2.3
1	B	354	VAL	2.3
1	A	77	ASN	2.3
1	B	259	LEU	2.3
1	A	132	GLY	2.2
1	A	241	THR	2.2
1	A	69	GLY	2.2
1	B	347	ASP	2.1
1	B	189	LYS	2.1
1	A	369	ILE	2.1
1	A	75	VAL	2.1
1	A	300	ALA	2.1
1	B	216	LEU	2.1
1	A	81	ILE	2.1
1	B	70	GLU	2.1
1	B	369	ILE	2.1
1	A	261	PHE	2.1
1	B	301	ASN	2.1
1	A	62	LEU	2.0
1	A	243	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 [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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	GDP	B	900	28/28	0.93	0.17	1.20	38,55,67,79	0
2	GDP	A	900	28/28	0.89	0.20	0.37	40,59,74,82	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.