



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:23 AM UTC

PDB ID : 3EC1 / pdb_00003ec1
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

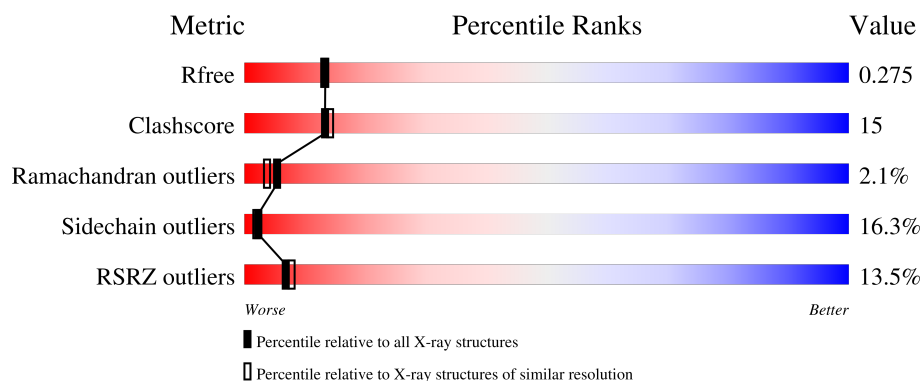
1 Overall quality at a glance

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}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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 $\leq 5\%$. 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	
1	B	369	

2 Entry composition [i](#)

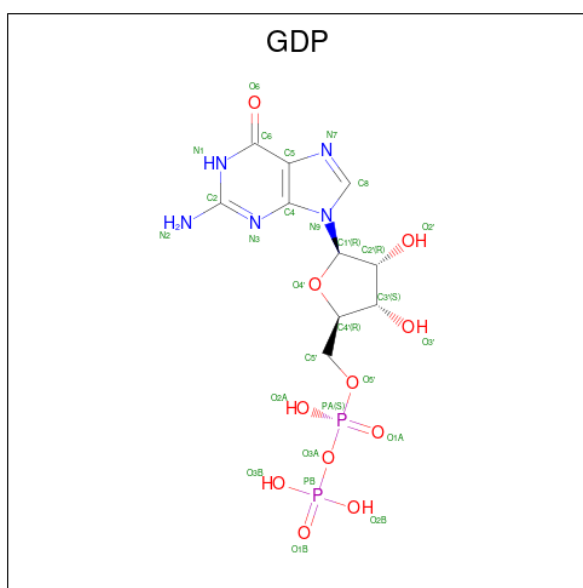
There are 3 unique types of molecules in this entry. The entry contains 5245 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 GTP-binding protein YqeH required for biosis of 30S ribosome subunit.

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 (CCD ID: 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		

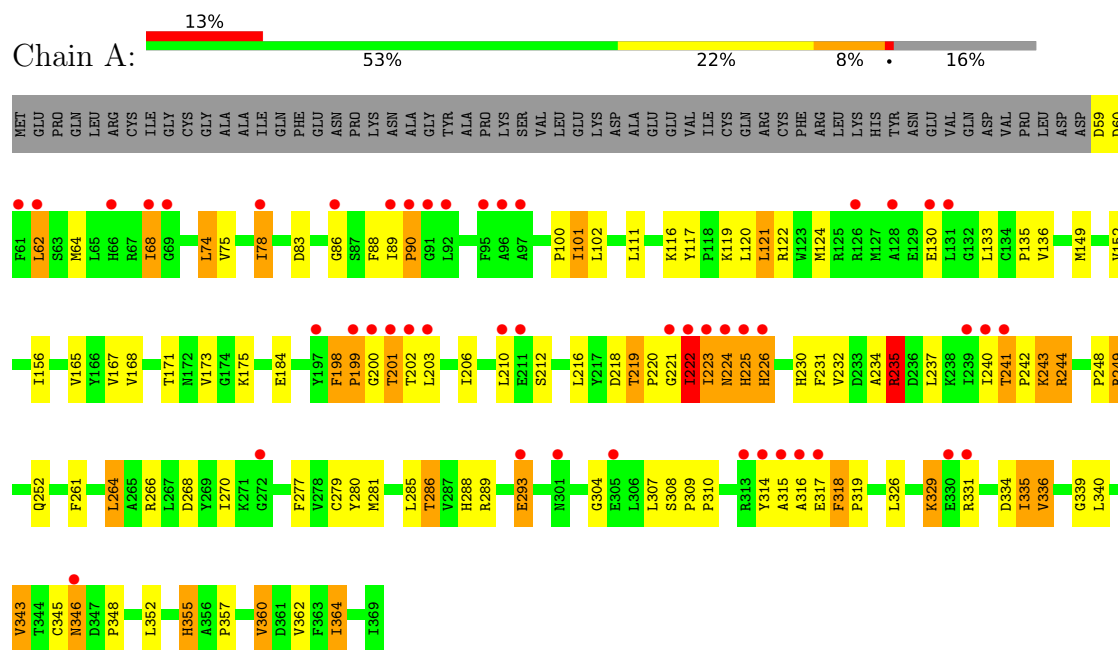
- Molecule 3 is water.

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

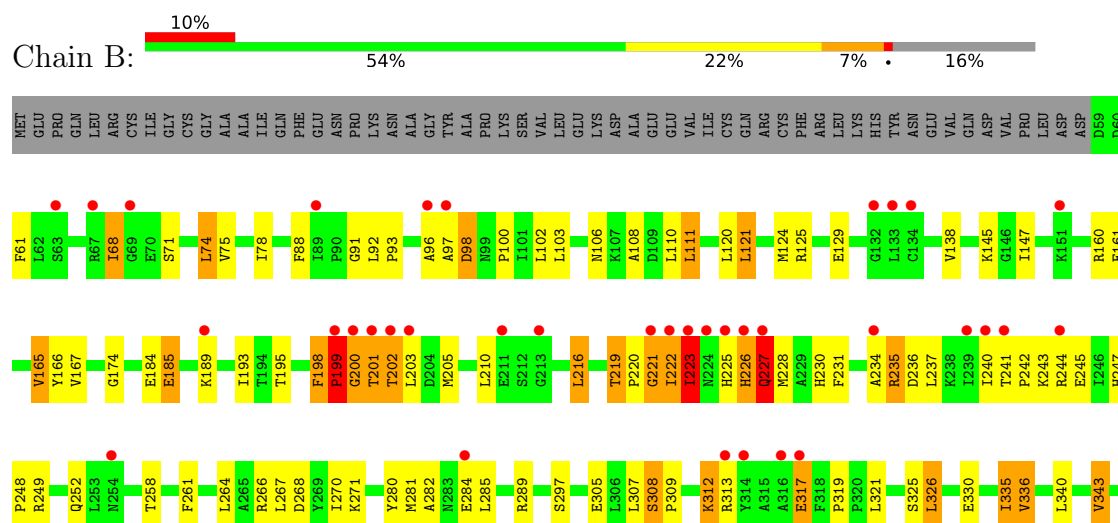
3 Residue-property plots

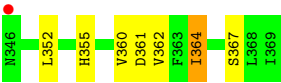
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: GTP-binding protein YqeH required for biosis of 30S ribosome subunit



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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	47.62Å 81.10Å 108.17Å 90.00° 91.50° 90.00°	Depositor
Resolution (Å)	30.00 – 2.36 30.00 – 2.36	Depositor EDS
% Data completeness (in resolution range)	99.4 (30.00-2.36) 95.0 (30.00-2.36)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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	1682 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	41.9	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 70.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.032 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5245	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹ Intensities estimated from amplitudes.

² Theoretical 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

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	0.52	1/2479 (0.0%)	1.07	13/3358 (0.4%)
1	B	0.49	1/2479 (0.0%)	1.09	19/3358 (0.6%)
All	All	0.50	2/4958 (0.0%)	1.08	32/6716 (0.5%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	PHE	CA-C	6.79	1.60	1.52
1	B	198	PHE	CA-C	5.75	1.60	1.53

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	PHE	N-CA-C	-10.38	96.58	109.65
1	B	198	PHE	N-CA-C	-9.05	98.70	109.93
1	B	210	LEU	N-CA-C	-7.98	98.12	110.17
1	B	199	PRO	N-CA-C	7.47	127.85	112.47
1	A	318	PHE	CA-C-N	7.45	125.10	119.66
1	A	318	PHE	C-N-CA	7.45	125.10	119.66
1	A	198	PHE	CA-C-N	6.83	128.38	119.84
1	A	198	PHE	C-N-CA	6.83	128.38	119.84
1	B	71	SER	N-CA-C	-6.64	99.70	110.20
1	A	210	LEU	N-CA-C	-6.47	100.63	110.14
1	B	91	GLY	N-CA-C	-6.47	106.78	114.48
1	A	212	SER	N-CA-C	6.26	119.88	111.24
1	A	315	ALA	N-CA-C	-6.21	105.76	113.15
1	B	221	GLY	N-CA-C	-6.16	105.34	112.73
1	B	200	GLY	N-CA-C	-6.13	98.64	113.18
1	A	336	VAL	N-CA-C	5.95	117.33	108.23
1	B	270	ILE	N-CA-C	5.85	116.06	110.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	336	VAL	N-CA-C	5.81	117.12	108.23
1	A	270	ILE	N-CA-C	5.73	115.81	110.42
1	A	203	LEU	N-CA-C	5.64	117.42	108.67
1	B	160	ARG	N-CA-C	-5.63	106.25	113.23
1	B	125	ARG	N-CA-C	-5.58	105.11	111.07
1	B	223	ILE	N-CA-C	-5.57	97.76	109.34
1	A	101	ILE	N-CA-C	5.50	115.82	108.11
1	B	335	ILE	N-CA-C	-5.29	98.84	106.88
1	B	98	ASP	N-CA-C	-5.25	106.87	113.28
1	B	202	THR	N-CA-C	-5.21	103.73	110.19
1	B	228	MET	N-CA-C	5.18	117.60	111.33
1	B	367	SER	N-CA-C	5.17	116.95	110.24
1	B	236	ASP	N-CA-C	-5.09	107.46	113.97
1	B	361	ASP	N-CA-C	5.07	117.56	109.96
1	A	335	ILE	N-CA-C	-5.01	99.27	106.88

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	84	0
1	B	2427	0	2474	60	0
2	A	28	0	12	0	0
2	B	28	0	12	4	0
3	A	167	0	0	3	0
3	B	168	0	0	2	0
All	All	5245	0	4972	146	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 15.

All (146) 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:H8	2:B:900:GDP:H5''	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:261:PHE:CD2	1:A:281:MET:HE1	2.24	0.73
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: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:O	1:A:89:ILE:HG22	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:261:PHE:CD2	1:B:281:MET:HE1	2.32	0.65
1:B:266:ARG:HD2	1:B:355:HIS:CD2	2.33	0.64
1:A:308:SER:HA	1:A:309:PRO:C	2.23	0.63
1:A:78:ILE:HG12	1:A:173:VAL:HG12	1.82	0.61
1:A:261:PHE:HD2	1:A:281:MET:HE1	1.63	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: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
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:A:279:CYS:SG	1:A:281:MET:HE2	2.46	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:A:314:TYR:C	1:A:316:ALA:H	2.14	0.55
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:308:SER:HA	1:B:309:PRO:C	2.34	0.51
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:89:ILE:O	1:A:90:PRO:C	2.54	0.50
1:B:335:ILE:HD12	1:B:343:VAL:HG22	1.93	0.50
1:B:88:PHE:O	1:B:225:HIS:CE1	2.64	0.50
1:B:201:THR:CG2	1:B:202:THR:N	2.75	0.50
1:A:86:GLY:C	1:A:225:HIS:CE1	2.90	0.50
1:A:248:PRO:HG3	1:A:280:TYR:HE1	1.77	0.50
1:B:68:ILE:HD13	1:B:166:TYR:CD1	2.46	0.50
1:A:222:ILE:O	1:A:223:ILE:CB	2.60	0.49
1:A:249:ARG:HD3	3:A:982:HOH:O	2.12	0.49
1:B:68:ILE:HD11	1:B:75:VAL:HG22	1.94	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:HA	1:B:313:ARG:HE	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:HD12	1:B:68:ILE:O	2.14	0.48
1:B:313:ARG:HA	1:B:313:ARG:NE	2.29	0.47
1:A:252:GLN:O	1:A:289:ARG:NH2	2.42	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:243:LYS:C	1:A:244:ARG:HG3	2.40	0.46
1:A:329:LYS:NZ	1:A:329:LYS:HB3	2.30	0.46
1:A:357:PRO:O	1:A:360:VAL:HG13	2.15	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: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:B:261:PHE:HD2	1:B:281:MET:HE1	1.77	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:220:PRO:C	1:A:222:ILE:N	2.74	0.44
1:A:219:THR:HG23	1:A:220:PRO:CD	2.45	0.44
1:A:220:PRO:C	1:A:222:ILE:H	2.25	0.44
1:A:277:PHE:CE1	1:A:345:CYS:SG	3.09	0.44
1:A:304:GLY:HA2	1:A:310:PRO:O	2.17	0.44
1:A:346:ASN:ND2	1:A:346:ASN:H	2.15	0.44
1:A:206:ILE:HB	1:A:218:ASP:HB3	2.00	0.44
1:A:88:PHE:C	1:A:90:PRO:HD2	2.42	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:B:267:LEU:HD23	1:B:267:LEU:C	2.42	0.44
1:A:152:VAL:O	1:A:156:ILE:HG13	2.18	0.44
1:A:335:ILE:HD12	1:A:343:VAL:HG22	1.99	0.44
1:A:88:PHE:O	1:A:90:PRO:HD2	2.18	0.43
1:A:74:LEU:HA	1:A:100:PRO:HG2	2.01	0.43
1:B:336:VAL:O	1:B:362:VAL:HA	2.18	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:A:116:LYS:HB2	1:A:119:LYS:HG3	2.01	0.43
1:B:222:ILE:O	1:B:223:ILE:HG13	2.19	0.43
1:B:326:LEU:HG	1:B:364:ILE:HG22	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:LEU:O	1:B:124:MET:HG2	2.19	0.42
1:A:117:TYR:O	1:A:121:LEU:HB2	2.20	0.42
1:B:258:THR:O	1:B:289:ARG:HA	2.19	0.41
1:B:74:LEU:HA	1:B:100:PRO:HG2	2.02	0.41
1:B:242:PRO:HG3	1:B:282:ALA:HB2	2.02	0.41
1:A:241:THR:HA	1:A:242:PRO:HD3	1.87	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: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:B:201:THR:C	1:B:202:THR:O	2.62	0.41
1:A:89:ILE:O	1:A:89:ILE:CG2	2.63	0.41
1:A:240:ILE:HD11	1:A:264:LEU:HD21	2.01	0.40
1:B:111:LEU:O	1:B:245:GLU:HG3	2.21	0.40
1:B:247:HIS:HA	1:B:248:PRO:HD3	1.94	0.40
1:A:68:ILE:HD11	1:A:75:VAL:CG2	2.51	0.40
1:A:149:MET:O	1:A:152:VAL:HG12	2.20	0.40
1:A:175:LYS:HE3	1:A:221:GLY:HA2	2.04	0.40
1:A:83:ASP:HB2	1:A:339:GLY:HA2	2.03	0.40
1:A:198:PHE:C	1:A:200:GLY:H	2.27	0.40
1:B:61:PHE:CE2	1:B:222:ILE:O	2.74	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	309/369 (84%)	284 (92%)	19 (6%)	6 (2%)	6	5
1	B	309/369 (84%)	286 (93%)	16 (5%)	7 (2%)	5	3
All	All	618/738 (84%)	570 (92%)	35 (6%)	13 (2%)	5	4

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%)	220 (83%)	44 (17%)	2	2
1	B	264/314 (84%)	222 (84%)	42 (16%)	2	2
All	All	528/628 (84%)	442 (84%)	86 (16%)	2	2

All (86) 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
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

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Mol	Chain	Res	Type
1	A	130	GLU
1	A	136	VAL
1	A	165	VAL
1	A	168	VAL
1	A	184	GLU
1	A	199	PRO
1	A	216	LEU
1	A	219	THR
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	241	THR
1	A	243	LYS
1	A	244	ARG
1	A	249	ARG
1	A	264	LEU
1	A	285	LEU
1	A	286	THR
1	A	293	GLU
1	A	307	LEU
1	A	317	GLU
1	A	326	LEU
1	A	329	LYS
1	A	340	LEU
1	A	343	VAL
1	A	346	ASN
1	A	352	LEU
1	A	355	HIS
1	A	360	VAL
1	A	364	ILE
1	B	68	ILE
1	B	74	LEU
1	B	78	ILE
1	B	98	ASP
1	B	102	LEU
1	B	103	LEU
1	B	111	LEU
1	B	121	LEU

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Mol	Chain	Res	Type
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	219	THR
1	B	226	HIS
1	B	227	GLN
1	B	237	LEU
1	B	240	ILE
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	305	GLU
1	B	307	LEU
1	B	308	SER
1	B	312	LYS
1	B	317	GLU
1	B	321	LEU
1	B	326	LEU
1	B	330	GLU
1	B	340	LEU
1	B	343	VAL
1	B	352	LEU
1	B	360	VAL
1	B	364	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	172	ASN
1	A	224	ASN
1	A	225	HIS
1	A	227	GLN

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Mol	Chain	Res	Type
1	A	252	GLN
1	A	301	ASN
1	A	302	GLN
1	A	346	ASN
1	A	366	GLN
1	B	85	ASN
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 oligosaccharides 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	B	900	-	29,30,30	1.27	3 (10%)	45,47,47	2.98	23 (51%)
2	GDP	A	900	-	29,30,30	0.99	0	45,47,47	2.24	15 (33%)

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	B	900	-	-	0/16/32/32	0/3/3/3
2	GDP	A	900	-	-	0/16/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	900	GDP	O4'-C1'	3.31	1.49	1.42
2	B	900	GDP	PA-O3A	2.60	1.62	1.59
2	B	900	GDP	PB-O3B	2.24	1.63	1.54

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	900	GDP	O2B-PB-O3A	-6.86	81.62	104.64
2	A	900	GDP	O5'-PA-O1A	-6.10	84.76	108.94
2	B	900	GDP	O2A-PA-O5'	-6.08	80.02	107.57
2	B	900	GDP	O5'-PA-O1A	-6.01	85.10	108.94
2	B	900	GDP	O3B-PB-O3A	-5.65	85.68	104.64
2	B	900	GDP	C2-N3-C4	5.40	121.60	112.30
2	A	900	GDP	O2A-PA-O5'	-5.38	83.20	107.57
2	B	900	GDP	C5-C4-N3	-5.37	119.84	128.39
2	A	900	GDP	C5-C4-N3	-5.18	120.14	128.39
2	A	900	GDP	C2-N3-C4	5.04	120.98	112.30
2	B	900	GDP	O3A-PB-O1B	-4.71	86.24	111.04
2	B	900	GDP	O3A-PA-O1A	4.59	124.52	110.70
2	B	900	GDP	C2'-C1'-N9	-4.30	101.29	113.25
2	B	900	GDP	O4'-C1'-N9	4.28	118.06	108.36
2	A	900	GDP	O2A-PA-O3A	4.01	118.10	107.27
2	A	900	GDP	N9-C4-N3	3.97	133.89	125.95
2	B	900	GDP	N9-C4-N3	3.60	133.15	125.95
2	B	900	GDP	C2'-C3'-C4'	3.31	109.01	102.61
2	B	900	GDP	O2B-PB-O1B	3.21	123.36	110.83
2	A	900	GDP	O4'-C4'-C3'	2.91	110.93	105.15
2	B	900	GDP	C2-N1-C6	-2.83	119.97	125.11
2	A	900	GDP	O3A-PA-O1A	2.83	119.22	110.70
2	B	900	GDP	C8-N7-C5	2.79	109.22	104.26
2	A	900	GDP	C8-N7-C5	2.69	109.06	104.26
2	B	900	GDP	O3B-PB-O2B	2.52	117.25	107.80
2	A	900	GDP	PA-O5'-C5'	-2.46	107.23	121.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	900	GDP	C6-C5-N7	2.43	134.71	130.29
2	A	900	GDP	C2-N1-C6	-2.41	120.74	125.11
2	B	900	GDP	C4-C5-N7	-2.29	107.04	110.67
2	A	900	GDP	C3'-C2'-C1'	2.28	105.77	101.46
2	B	900	GDP	C3'-C2'-C1'	2.19	105.60	101.46
2	A	900	GDP	O6-C6-C5	-2.18	120.77	126.53
2	A	900	GDP	C6-C5-N7	2.15	134.21	130.29
2	B	900	GDP	C5-C6-N1	2.11	118.64	113.25
2	B	900	GDP	O6-C6-C5	-2.09	121.02	126.53
2	B	900	GDP	O4'-C4'-C5'	-2.06	102.73	109.33
2	B	900	GDP	O2A-PA-O3A	2.04	112.80	107.27
2	A	900	GDP	C5-C6-N1	2.01	118.37	113.25

There are no chirality outliers.

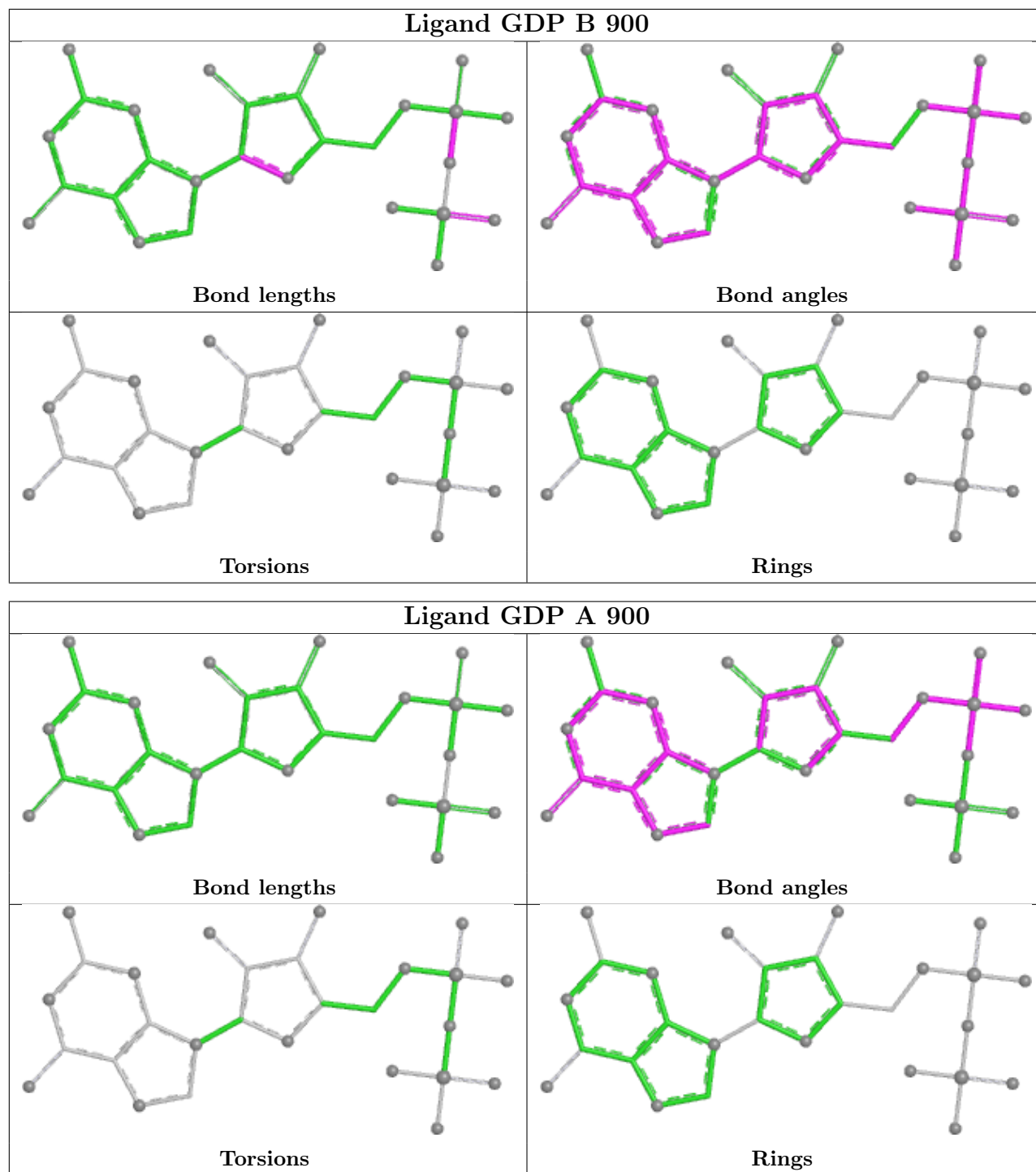
There are no torsion outliers.

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

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 ⓘ

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, 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	311/369 (84%)	0.86	47 (15%) 5 6	17, 42, 79, 95	0
1	B	311/369 (84%)	0.80	37 (11%) 9 10	20, 43, 77, 92	0
All	All	622/738 (84%)	0.83	84 (13%) 7 8	17, 42, 78, 95	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	221	GLY	11.7
1	B	222	ILE	7.8
1	A	222	ILE	6.2
1	B	201	THR	6.1
1	A	317	GLU	5.9
1	A	200	GLY	5.4
1	A	202	THR	5.4
1	A	201	THR	5.2
1	A	225	HIS	5.1
1	B	221	GLY	4.9
1	A	315	ALA	4.5
1	A	316	ALA	4.5
1	B	226	HIS	4.4
1	B	223	ILE	4.3
1	B	284	GLU	4.0
1	B	240	ILE	4.0
1	B	316	ALA	4.0
1	B	200	GLY	4.0
1	B	132	GLY	3.8
1	B	202	THR	3.7
1	B	346	ASN	3.7
1	B	67	ARG	3.7
1	A	223	ILE	3.6
1	A	314	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	203	LEU	3.5
1	A	330	GLU	3.5
1	A	346	ASN	3.4
1	A	241	THR	3.3
1	B	317	GLU	3.3
1	A	203	LEU	3.3
1	A	272	GLY	3.3
1	A	131	LEU	3.2
1	A	240	ILE	3.2
1	B	199	PRO	3.2
1	A	331	ARG	3.1
1	A	69	GLY	3.1
1	A	86	GLY	3.1
1	B	239	ILE	3.1
1	B	213	GLY	3.1
1	B	225	HIS	3.0
1	B	254	ASN	2.9
1	A	89	ILE	2.9
1	B	69	GLY	2.8
1	A	95	PHE	2.8
1	B	241	THR	2.8
1	A	199	PRO	2.7
1	B	134	CYS	2.7
1	A	293	GLU	2.7
1	B	151	LYS	2.7
1	B	313	ARG	2.7
1	A	91	GLY	2.6
1	A	92	LEU	2.6
1	B	133	LEU	2.6
1	A	126	ARG	2.6
1	A	239	ILE	2.5
1	A	130	GLU	2.4
1	A	226	HIS	2.4
1	A	211	GLU	2.4
1	B	211	GLU	2.4
1	A	97	ALA	2.4
1	B	63	SER	2.4
1	B	97	ALA	2.3
1	A	61	PHE	2.3
1	A	313	ARG	2.3
1	A	62	LEU	2.3
1	A	197	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	128	ALA	2.2
1	A	301	ASN	2.2
1	A	68	ILE	2.2
1	B	96	ALA	2.2
1	B	314	TYR	2.2
1	A	66	HIS	2.2
1	A	210	LEU	2.1
1	B	234	ALA	2.1
1	B	227	GLN	2.1
1	B	244	ARG	2.1
1	A	305	GLU	2.1
1	A	78	ILE	2.1
1	B	89	ILE	2.1
1	B	224	ASN	2.1
1	A	90	PRO	2.0
1	B	189	LYS	2.0
1	A	96	ALA	2.0
1	A	224	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 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.

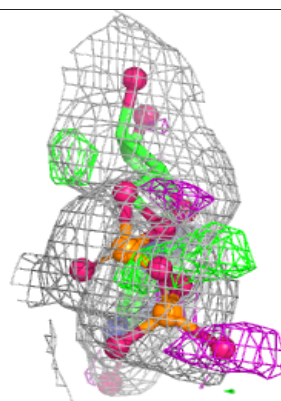
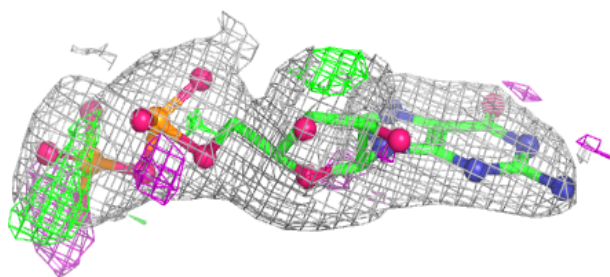
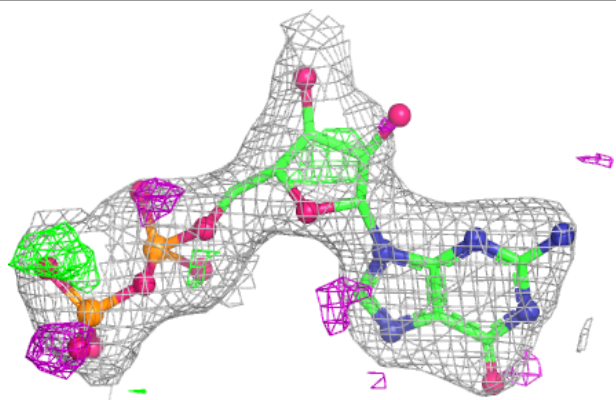
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GDP	A	900	28/28	0.86	0.15	40,59,74,82	0
2	GDP	B	900	28/28	0.89	0.13	38,55,67,79	0

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.

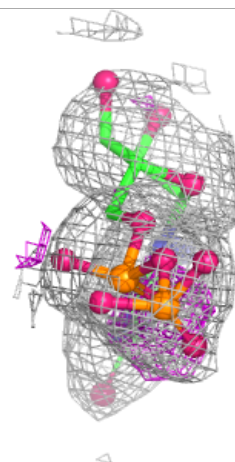
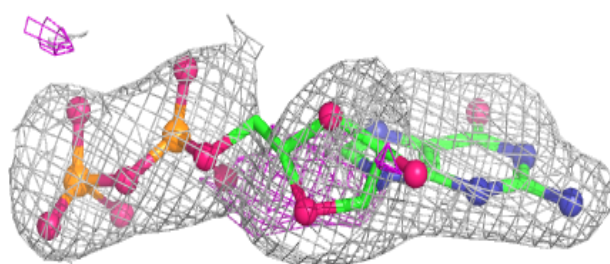
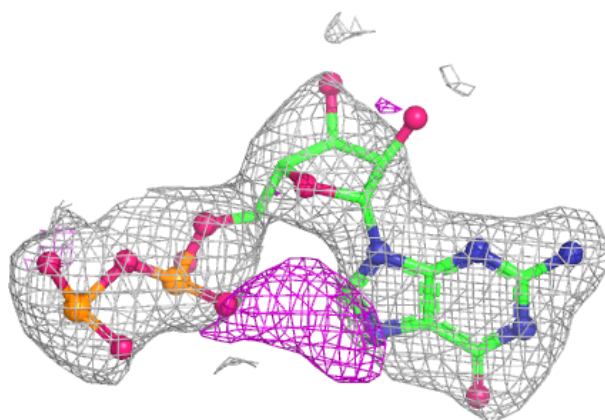
Electron density around GDP A 900:

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



Electron density around GDP B 900:

$2mF_o-DF_c$ (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.