



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 07:48 PM UTC

PDB ID : 2RHL / pdb_00002rhl
Title : Synthetic Gene Encoded Bacillus Subtilis FtsZ NCS Dimer with Bound GDP
Authors : Lovell, S.; Halloran, Z.; Hjerrild, K.; Sheridan, D.; Burgin, A.; Stewart, L.;
Accelerated Technologies Center for Gene to 3D Structure (ATCG3D)
Deposited on : 2007-10-09
Resolution : 2.45 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

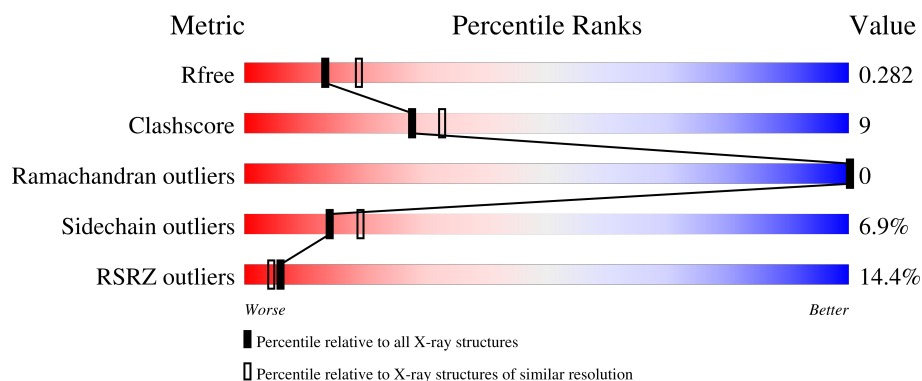
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	325	14% 75% 16% • 6%
1	B	325	14% 78% 18% • •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4642 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 Cell Division Protein ftsZ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	305	Total	C	N	O	S	0	0	0
			2199	1369	379	441	10			
1	B	315	Total	C	N	O	S	0	0	0
			2290	1427	397	456	10			

There are 42 discrepancies between the modelled and reference sequences:

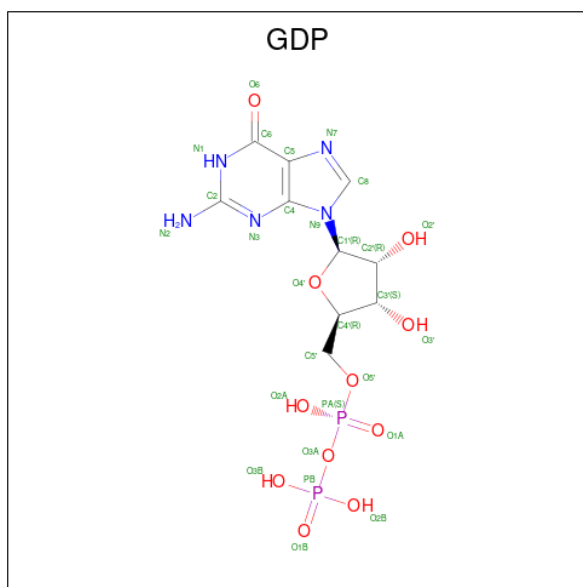
Chain	Residue	Modelled	Actual	Comment	Reference
A	11	MET	-	expression tag	UNP P17865
A	316	LEU	-	expression tag	UNP P17865
A	317	GLU	-	expression tag	UNP P17865
A	318	ASN	-	expression tag	UNP P17865
A	319	LEU	-	expression tag	UNP P17865
A	320	TYR	-	expression tag	UNP P17865
A	321	PHE	-	expression tag	UNP P17865
A	322	GLN	-	expression tag	UNP P17865
A	323	GLY	-	expression tag	UNP P17865
A	324	HIS	-	expression tag	UNP P17865
A	325	HIS	-	expression tag	UNP P17865
A	326	HIS	-	expression tag	UNP P17865
A	327	HIS	-	expression tag	UNP P17865
A	328	HIS	-	expression tag	UNP P17865
A	329	HIS	-	expression tag	UNP P17865
A	330	GLU	-	expression tag	UNP P17865
A	331	TYR	-	expression tag	UNP P17865
A	332	MET	-	expression tag	UNP P17865
A	333	PRO	-	expression tag	UNP P17865
A	334	MET	-	expression tag	UNP P17865
A	335	GLU	-	expression tag	UNP P17865
B	11	MET	-	expression tag	UNP P17865
B	316	LEU	-	expression tag	UNP P17865
B	317	GLU	-	expression tag	UNP P17865
B	318	ASN	-	expression tag	UNP P17865

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	319	LEU	-	expression tag	UNP P17865
B	320	TYR	-	expression tag	UNP P17865
B	321	PHE	-	expression tag	UNP P17865
B	322	GLN	-	expression tag	UNP P17865
B	323	GLY	-	expression tag	UNP P17865
B	324	HIS	-	expression tag	UNP P17865
B	325	HIS	-	expression tag	UNP P17865
B	326	HIS	-	expression tag	UNP P17865
B	327	HIS	-	expression tag	UNP P17865
B	328	HIS	-	expression tag	UNP P17865
B	329	HIS	-	expression tag	UNP P17865
B	330	GLU	-	expression tag	UNP P17865
B	331	TYR	-	expression tag	UNP P17865
B	332	MET	-	expression tag	UNP P17865
B	333	PRO	-	expression tag	UNP P17865
B	334	MET	-	expression tag	UNP P17865
B	335	GLU	-	expression tag	UNP P17865

- 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		

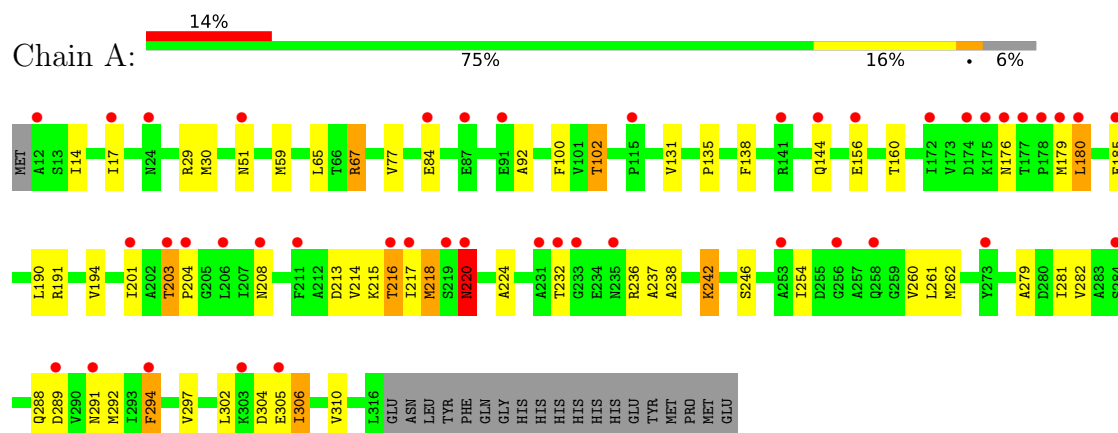
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	51	Total 51	O 51	0	0
3	B	46	Total 46	O 46	0	0

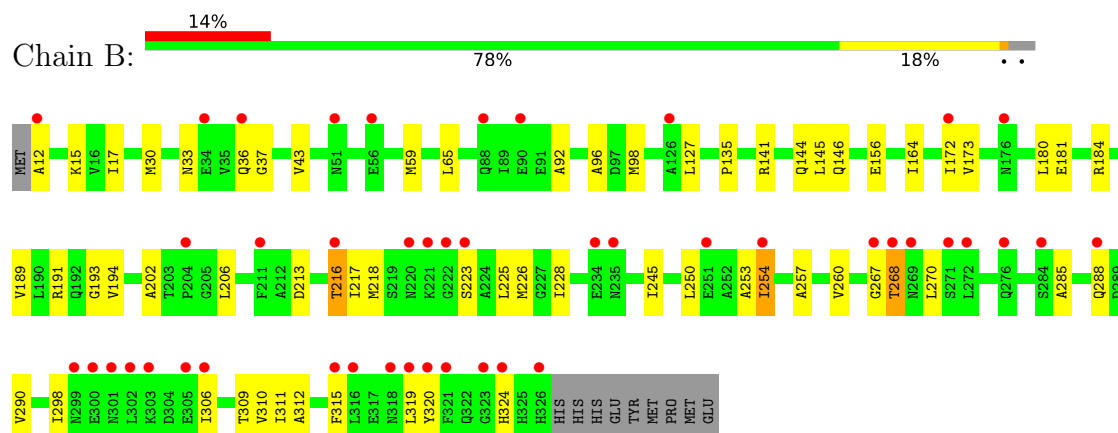
3 Residue-property plots

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: Cell Division Protein ftsZ



• Molecule 1: Cell Division Protein ftsZ



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.29Å 97.58Å 135.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.45 30.00 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.0 (30.00-2.45) 98.9 (30.00-2.45)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.77 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.227 , 0.270 0.233 , 0.282	Depositor DCC
R_{free} test set	2039 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	54.2	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4642	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.34% 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

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	0.92	2/2214 (0.1%)	0.98	1/2991 (0.0%)
1	B	0.92	0/2310	0.93	0/3121
All	All	0.92	2/4524 (0.0%)	0.96	1/6112 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	218	MET	CA-C	-5.42	1.47	1.53
1	A	77	VAL	CA-CB	5.06	1.60	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	294	PHE	N-CA-C	7.26	120.11	109.07

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	220	ASN	Peptide

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	2199	0	2257	38	0
1	B	2290	0	2330	47	0
2	A	28	0	12	0	0
2	B	28	0	12	0	0
3	A	51	0	0	2	0
3	B	46	0	0	3	0
All	All	4642	0	4611	82	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 9.

All (82) 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:84:GLU:OE1	3:A:354:HOH:O	1.67	1.12
1:B:217:ILE:HD11	1:B:218:MET:HE2	1.54	0.89
1:B:225:LEU:HD12	1:B:315:PHE:CE2	2.13	0.83
1:B:193:GLY:HA2	1:B:226:MET:HE1	1.67	0.76
1:B:225:LEU:CD1	1:B:315:PHE:CE2	2.69	0.76
1:A:59:MET:HE1	1:A:92:ALA:CB	2.16	0.75
1:A:201:ILE:HD11	1:A:214:VAL:HG21	1.69	0.74
1:A:67:ARG:HH22	1:B:146:GLN:HE22	1.40	0.68
1:B:223:SER:HA	3:B:339:HOH:O	1.94	0.67
1:A:237:ALA:HA	1:A:306:ILE:HD11	1.76	0.67
1:B:30:MET:HG2	1:B:191:ARG:HG3	1.79	0.65
1:A:213:ASP:O	1:A:216:THR:HB	1.98	0.64
1:B:135:PRO:O	1:B:144:GLN:NE2	2.31	0.64
1:B:193:GLY:HA2	1:B:226:MET:CE	2.28	0.63
1:B:181:GLU:OE1	1:B:184:ARG:HD3	1.98	0.62
1:B:206:LEU:HD11	1:B:270:LEU:O	1.99	0.62
1:B:59:MET:HE1	1:B:92:ALA:CB	2.30	0.61
1:B:17:ILE:HD11	1:B:43:VAL:HG21	1.83	0.60
1:A:254:ILE:HD12	1:A:310:VAL:HG11	1.84	0.60
1:B:268:THR:HA	1:B:298:ILE:HD12	1.84	0.59
1:B:254:ILE:HD12	1:B:310:VAL:HG11	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:ILE:CD1	1:A:310:VAL:HG11	2.32	0.58
1:B:17:ILE:HD11	1:B:43:VAL:CG2	2.36	0.56
1:B:193:GLY:CA	1:B:226:MET:HE1	2.34	0.56
1:B:257:ALA:HB2	1:B:312:ALA:HB1	1.87	0.56
1:B:226:MET:HE3	1:B:311:ILE:HD11	1.88	0.56
1:A:215:LYS:NZ	3:A:366:HOH:O	2.37	0.55
1:B:15:LYS:HD2	1:B:96:ALA:HB2	1.88	0.55
1:A:216:THR:HG22	1:A:217:ILE:HG23	1.89	0.53
1:B:253:ALA:O	1:B:315:PHE:HZ	1.92	0.53
1:A:302:LEU:HD22	1:A:305:GLU:HB3	1.90	0.53
1:B:59:MET:HE1	1:B:92:ALA:HB2	1.90	0.53
1:A:238:ALA:HA	1:A:281:ILE:CD1	2.39	0.52
1:A:261:LEU:C	1:A:261:LEU:HD23	2.35	0.52
1:B:12:ALA:O	3:B:358:HOH:O	2.19	0.52
1:B:30:MET:HE1	1:B:194:VAL:HG11	1.90	0.52
1:A:160:THR:HG23	1:A:220:ASN:HB2	1.92	0.52
1:B:254:ILE:HG22	3:B:363:HOH:O	2.11	0.51
1:A:203:THR:HG22	1:A:204:PRO:HD2	1.93	0.51
1:B:245:ILE:HD12	1:B:285:ALA:HB2	1.92	0.51
1:A:59:MET:HE1	1:A:92:ALA:HB2	1.93	0.50
1:B:37:GLY:HA3	1:B:202:ALA:HB1	1.93	0.50
1:A:262:MET:SD	1:A:282:VAL:HG21	2.51	0.50
1:A:14:ILE:HD11	1:A:201:ILE:HG22	1.94	0.49
1:B:141:ARG:NH1	1:B:145:LEU:HD21	2.28	0.49
1:A:102:THR:HG22	1:A:190:LEU:HD22	1.94	0.48
1:B:98:MET:HE3	1:B:127:LEU:HD23	1.95	0.48
1:B:225:LEU:CD1	1:B:315:PHE:CZ	2.96	0.47
1:A:232:THR:HG22	1:A:304:ASP:C	2.39	0.47
1:B:267:GLY:C	1:B:298:ILE:HG23	2.39	0.47
1:A:236:ARG:HD2	1:A:306:ILE:HG23	1.95	0.47
1:A:67:ARG:HH22	1:B:146:GLN:NE2	2.10	0.46
1:B:226:MET:HE2	1:B:228:ILE:HD11	1.97	0.46
1:A:238:ALA:O	1:A:242:LYS:HB2	2.17	0.45
1:B:260:VAL:HG23	1:B:290:VAL:HG21	2.00	0.44
1:B:225:LEU:HD11	1:B:315:PHE:CE2	2.52	0.44
1:A:220:ASN:OD1	1:A:224:ALA:HB2	2.17	0.43
1:B:225:LEU:HD12	1:B:315:PHE:CZ	2.52	0.43
1:A:237:ALA:HA	1:A:306:ILE:CD1	2.45	0.43
1:A:216:THR:HG23	1:A:291:ASN:ND2	2.33	0.43
1:A:279:ALA:HB1	1:A:294:PHE:CZ	2.54	0.43
1:B:226:MET:HE2	1:B:309:THR:HG23	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:PRO:O	1:A:144:GLN:NE2	2.51	0.43
1:B:213:ASP:HA	1:B:216:THR:HG23	2.00	0.43
1:B:225:LEU:HD11	1:B:315:PHE:CZ	2.53	0.43
1:B:217:ILE:CD1	1:B:218:MET:HE2	2.36	0.42
1:B:193:GLY:N	1:B:226:MET:HE1	2.35	0.42
1:A:262:MET:HE2	1:A:294:PHE:CD1	2.54	0.42
1:B:33:ASN:HD22	1:B:33:ASN:N	2.16	0.42
1:A:292:MET:HE2	1:A:294:PHE:CE2	2.55	0.42
1:A:17:ILE:HG22	1:A:100:PHE:O	2.20	0.42
1:A:138:PHE:C	1:A:138:PHE:CD1	2.99	0.41
1:A:30:MET:HE1	1:A:194:VAL:HG11	2.03	0.41
1:A:102:THR:HG22	1:A:131:VAL:O	2.21	0.41
1:A:260:VAL:HG13	1:A:310:VAL:HG13	2.03	0.41
1:B:98:MET:HG3	1:B:127:LEU:HB3	2.02	0.41
1:B:164:ILE:HD13	1:B:189:VAL:HG12	2.03	0.41
1:B:320:TYR:CE1	1:B:324:HIS:CD2	3.08	0.41
1:A:65:LEU:HD11	1:B:65:LEU:HD11	2.01	0.41
1:B:141:ARG:HH12	1:B:145:LEU:HD21	1.85	0.41
1:A:238:ALA:HA	1:A:281:ILE:HD13	2.03	0.40
1:A:179:MET:O	1:A:180:LEU:C	2.65	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	303/325 (93%)	292 (96%)	11 (4%)	0	100	100
1	B	313/325 (96%)	307 (98%)	6 (2%)	0	100	100
All	All	616/650 (95%)	599 (97%)	17 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	227/246 (92%)	207 (91%)	20 (9%)	9	10
1	B	236/246 (96%)	224 (95%)	12 (5%)	21	31
All	All	463/492 (94%)	431 (93%)	32 (7%)	14	19

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ARG
1	A	51	ASN
1	A	67	ARG
1	A	102	THR
1	A	156	GLU
1	A	176	ASN
1	A	180	LEU
1	A	185	GLU
1	A	191	ARG
1	A	203	THR
1	A	208	ASN
1	A	216	THR
1	A	218	MET
1	A	220	ASN
1	A	242	LYS
1	A	246	SER
1	A	288	GLN
1	A	289	ASP
1	A	297	VAL
1	A	306	ILE
1	B	36	GLN
1	B	156	GLU
1	B	172	ILE
1	B	173	VAL
1	B	180	LEU
1	B	216	THR
1	B	250	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	254	ILE
1	B	268	THR
1	B	288	GLN
1	B	306	ILE
1	B	319	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	GLN
1	A	176	ASN
1	A	208	ASN
1	A	301	ASN
1	B	33	ASN
1	B	51	ASN
1	B	88	GLN
1	B	146	GLN
1	B	208	ASN
1	B	276	GLN
1	B	318	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 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	1	-	29,30,30	1.30	2 (6%)	45,47,47	1.96	9 (20%)
2	GDP	A	1	-	29,30,30	1.12	4 (13%)	45,47,47	1.75	9 (20%)

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	1	-	-	0/16/32/32	0/3/3/3
2	GDP	A	1	-	-	0/16/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	GDP	C5-C4	3.30	1.47	1.38
2	B	1	GDP	PA-O3A	-3.07	1.56	1.59
2	A	1	GDP	C5-C4	2.93	1.46	1.38
2	A	1	GDP	C5-N7	-2.18	1.34	1.39
2	A	1	GDP	C4-N9	-2.06	1.32	1.38
2	A	1	GDP	C6-N1	-2.05	1.35	1.38

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	GDP	C5-C4-N3	-5.88	119.03	128.39
2	B	1	GDP	C2-N3-C4	5.27	121.38	112.30
2	A	1	GDP	C2-N3-C4	4.95	120.83	112.30
2	B	1	GDP	C6-C5-N7	4.81	139.05	130.29
2	A	1	GDP	C5-C4-N3	-4.37	121.43	128.39
2	A	1	GDP	C6-C5-N7	4.08	137.72	130.29
2	B	1	GDP	C4-C5-N7	-3.88	104.52	110.67
2	B	1	GDP	N9-C4-N3	3.76	133.47	125.95
2	A	1	GDP	N9-C4-N3	3.23	132.42	125.95
2	A	1	GDP	O3B-PB-O3A	3.11	115.07	104.64
2	B	1	GDP	C8-N7-C5	2.96	109.54	104.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	GDP	C1'-N9-C4	-2.56	118.93	126.49
2	A	1	GDP	C6-C5-C4	-2.51	115.05	118.83
2	B	1	GDP	O3B-PB-O3A	2.41	112.70	104.64
2	B	1	GDP	N9-C8-N7	-2.38	108.99	113.40
2	A	1	GDP	C4-C5-N7	-2.17	107.24	110.67
2	B	1	GDP	C5-C6-N1	2.11	118.61	113.25
2	A	1	GDP	O6-C6-C5	-2.08	121.05	126.53

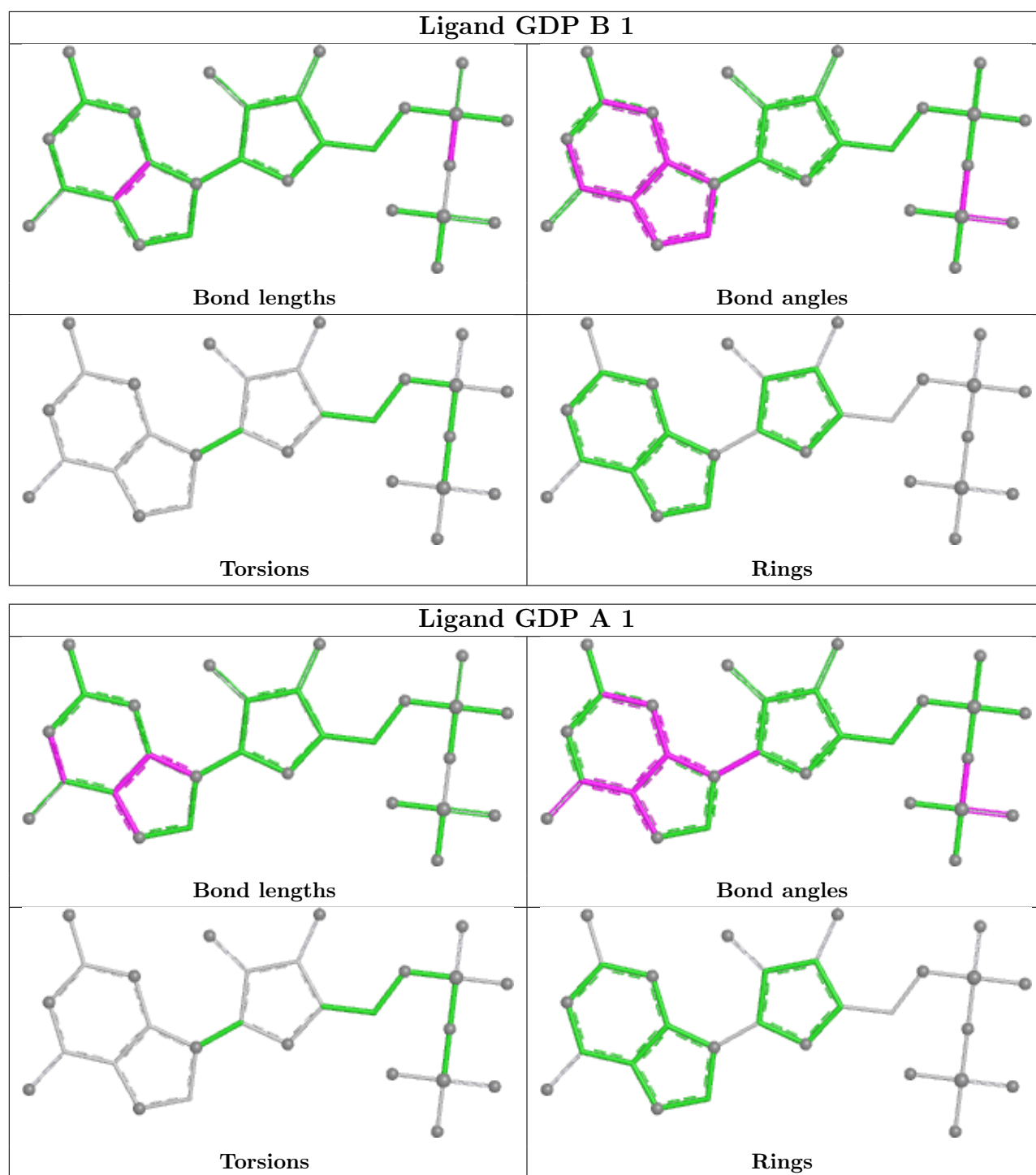
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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	305/325 (93%)	0.96	44 (14%) 6 4	50, 67, 84, 96	0
1	B	315/325 (96%)	0.87	45 (14%) 6 4	51, 65, 85, 100	0
All	All	620/650 (95%)	0.92	89 (14%) 6 4	50, 66, 85, 100	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	220	ASN	6.6
1	A	294	PHE	6.2
1	B	222	GLY	5.9
1	A	185	GLU	5.3
1	B	319	LEU	5.0
1	B	315	PHE	4.7
1	A	206	LEU	4.4
1	B	272	LEU	4.4
1	A	204	PRO	4.2
1	A	175	LYS	4.1
1	A	258	GLN	4.0
1	B	221	LYS	4.0
1	A	273	TYR	3.9
1	B	235	ASN	3.9
1	B	320	TYR	3.8
1	A	291	ASN	3.7
1	B	204	PRO	3.5
1	B	176	ASN	3.3
1	A	12	ALA	3.3
1	A	141	ARG	3.3
1	A	305	GLU	3.3
1	A	303	LYS	3.3
1	B	321	PHE	3.2
1	A	174	ASP	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	235	ASN	3.2
1	B	326	HIS	3.2
1	A	208	ASN	3.1
1	B	276	GLN	3.0
1	B	303	LYS	3.0
1	B	51	ASN	3.0
1	B	34	GLU	3.0
1	B	318	ASN	3.0
1	B	172	ILE	2.9
1	B	56	GLU	2.9
1	B	234	GLU	2.9
1	B	223	SER	2.9
1	A	176	ASN	2.9
1	B	324	HIS	2.9
1	A	180	LEU	2.9
1	B	316	LEU	2.9
1	B	288	GLN	2.8
1	B	12	ALA	2.8
1	B	268	THR	2.8
1	B	284	SER	2.7
1	B	269	ASN	2.7
1	A	203	THR	2.6
1	B	306	ILE	2.6
1	A	178	PRO	2.6
1	A	177	THR	2.6
1	A	219	SER	2.6
1	A	232	THR	2.5
1	B	126	ALA	2.5
1	A	216	THR	2.5
1	B	267	GLY	2.4
1	B	299	ASN	2.4
1	B	300	GLU	2.4
1	B	305	GLU	2.4
1	B	323	GLY	2.4
1	B	254	ILE	2.3
1	A	87	GLU	2.3
1	A	289	ASP	2.3
1	A	156	GLU	2.3
1	A	144	GLN	2.3
1	A	201	ILE	2.3
1	B	251	GLU	2.3
1	A	51	ASN	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	90	GLU	2.3
1	B	220	ASN	2.2
1	A	172	ILE	2.2
1	A	84	GLU	2.2
1	B	301	ASN	2.2
1	A	91	GLU	2.2
1	A	253	ALA	2.1
1	A	115	PRO	2.1
1	A	231	ALA	2.1
1	A	24	ASN	2.1
1	A	233	GLY	2.1
1	A	256	GLY	2.1
1	B	211	PHE	2.1
1	B	36	GLN	2.1
1	B	302	LEU	2.1
1	A	17	ILE	2.1
1	A	217	ILE	2.1
1	A	284	SER	2.1
1	B	88	GLN	2.1
1	B	271	SER	2.1
1	A	211	PHE	2.0
1	A	179	MET	2.0
1	B	216	THR	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.

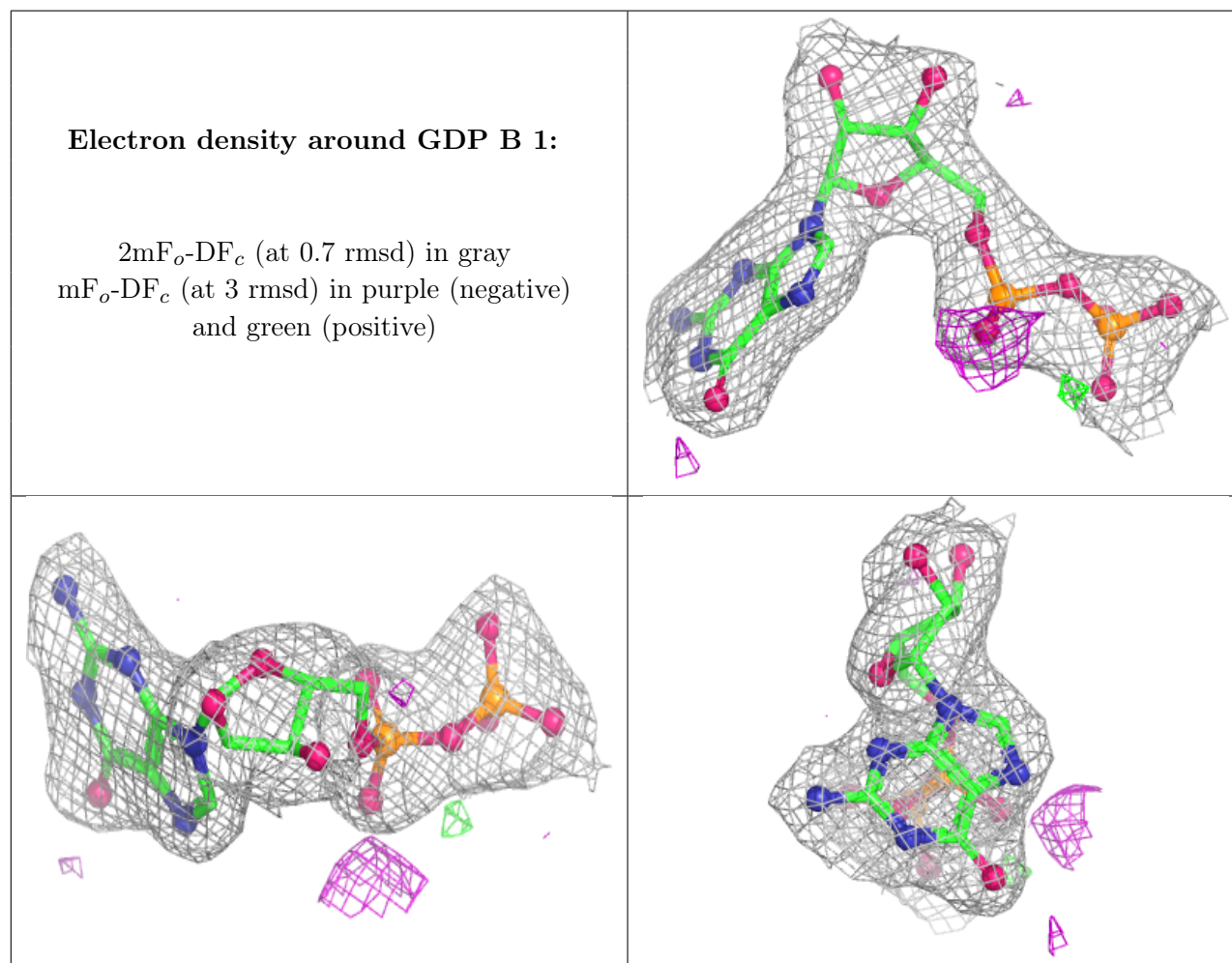
Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
-----	------	-------	-----	-------	------	-----	-----------------------------	-------

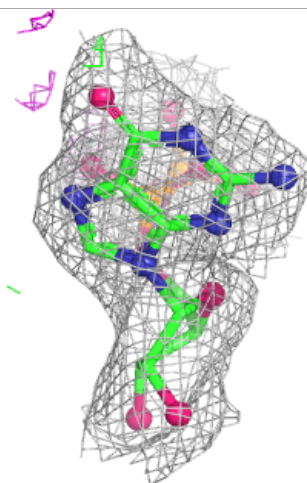
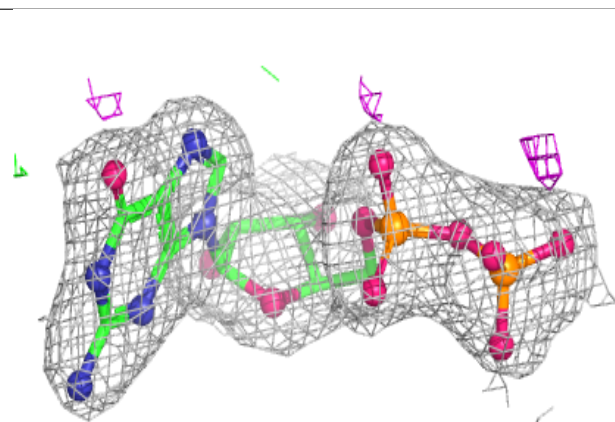
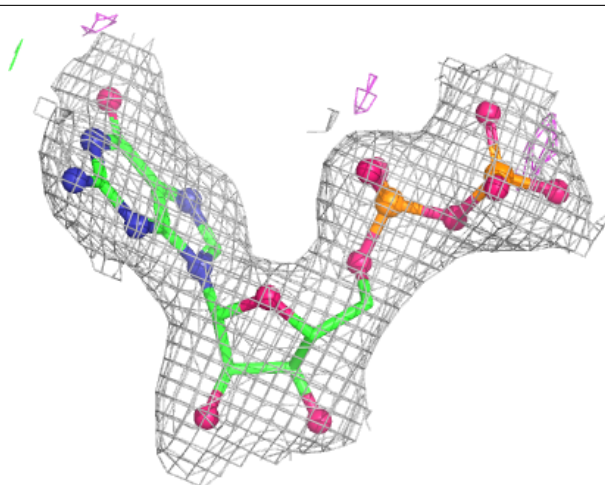
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GDP	B	1	28/28	0.97	0.07	50,52,55,56	0
2	GDP	A	1	28/28	0.98	0.06	49,59,62,63	0

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 1:

$2mF_o-DF_c$ (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.