



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:03 AM GMT

PDB ID : 3H2Y
Title : Crystal structure of YqeH GTPase from Bacillus anthracis with dGDP bound
Authors : Brunzelle, J.S.; Anderson, S.M.; Xu, X.; Savchenko, A.; Anderson, W.F.;
Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2009-04-15
Resolution : 1.80 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 ⓘ symbol.

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

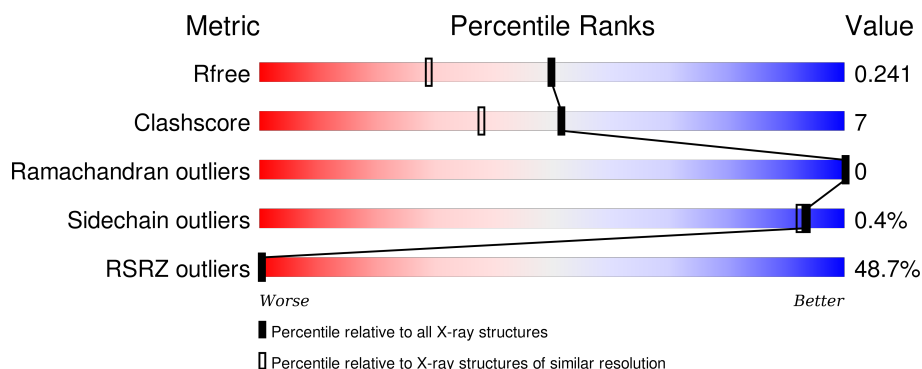
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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 $\leq 5\%$. 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	368	<div> <div>40%</div> <div>69%</div> <div>14%</div> <div>•</div> <div>16%</div> </div>

2 Entry composition [i](#)

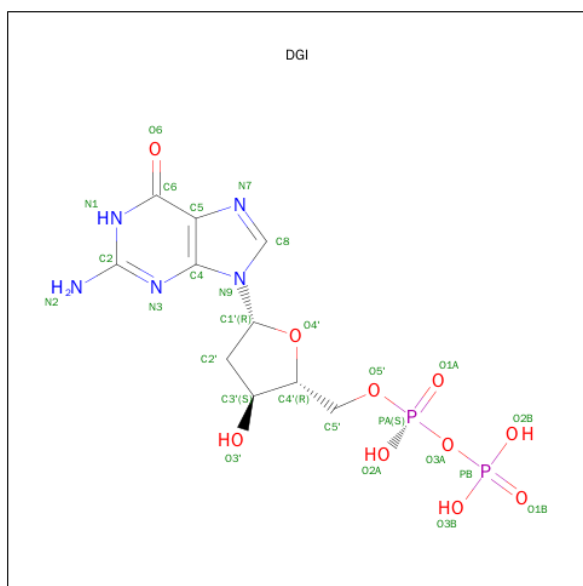
There are 3 unique types of molecules in this entry. The entry contains 2587 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 GTPase family protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	S	Se	17	2	0
			2434	1561	414	451	3	5			

- Molecule 2 is 2'-DEOXYGUANOSINE-5'-DIPHOSPHATE (three-letter code: DGI) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

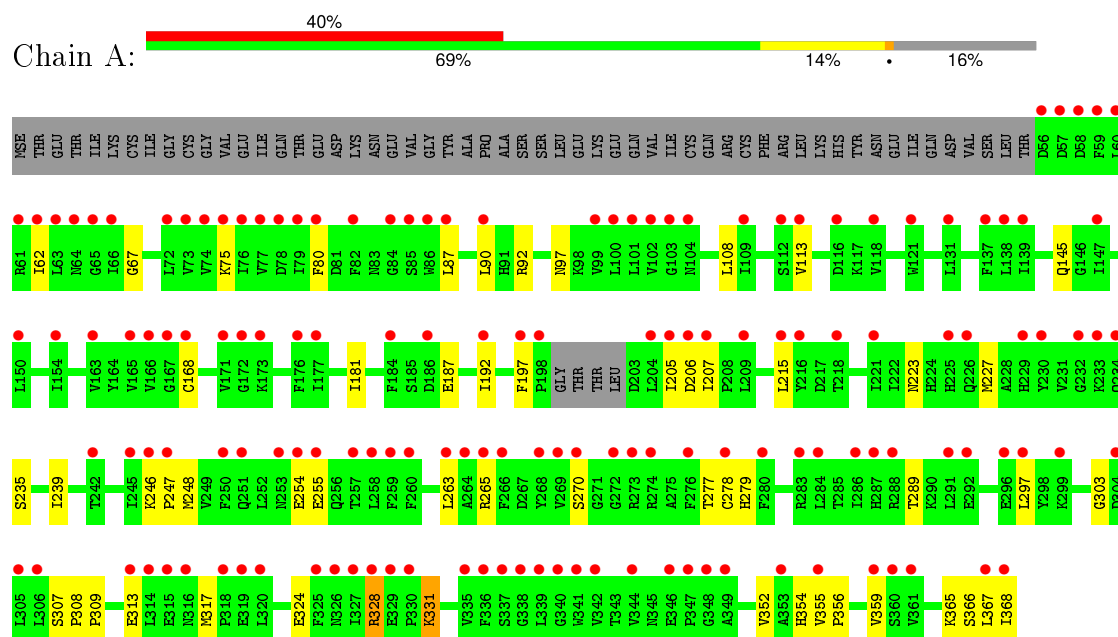
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	126	Total	O	0	0
			126	126		

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: GTPase family protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	83.13Å 58.99Å 77.72Å 90.00° 99.38° 90.00°	Depositor
Resolution (Å)	30.00 – 1.80 29.49 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.4 (30.00-1.80) 98.5 (29.49-1.80)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.67 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.215 , 0.242 0.213 , 0.241	Depositor DCC
R_{free} test set	1714 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	35.1	Xtriage
Anisotropy	0.546	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 58.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 34009 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	2587	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.47% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: DGI

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	0.48	2/2485 (0.1%)	0.63	5/3359 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	331	LYS	CG-CD	-10.30	1.17	1.52
1	A	328	ARG	CB-CG	-9.22	1.27	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	328	ARG	CA-CB-CG	8.76	132.68	113.40
1	A	331	LYS	CB-CG-CD	7.36	130.74	111.60
1	A	328	ARG	CB-CG-CD	5.89	126.92	111.60
1	A	365	LYS	CA-CB-CG	5.62	125.75	113.40
1	A	90	LEU	CA-CB-CG	5.25	127.37	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2434	0	2400	33	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	27	0	12	0	0
3	A	126	0	0	4	1
All	All	2587	0	2412	33	1

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 7.

All (33) 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:227:MSE:HE2	1:A:359:VAL:HG11	1.72	0.70
1:A:265:ARG:HB3	1:A:354:HIS:HB2	1.76	0.65
1:A:324:GLU:HG2	1:A:352:VAL:HG22	1.83	0.60
1:A:181:ILE:HD11	1:A:205:ILE:HD13	1.83	0.58
1:A:62:ILE:HG21	1:A:197:PHE:CE1	2.44	0.53
1:A:80:PHE:CE2	1:A:108:LEU:HB2	2.44	0.53
1:A:235:SER:O	1:A:239:ILE:HD12	2.09	0.53
1:A:355:VAL:HG22	1:A:356:PRO:HD2	1.93	0.50
1:A:355:VAL:HG22	1:A:359:VAL:HB	1.95	0.49
1:A:168[B]:CYS:SG	1:A:223:ASN:ND2	2.85	0.49
1:A:207:ILE:HD12	1:A:215:LEU:HD22	1.95	0.48
1:A:254:GLU:HG2	1:A:255:GLU:HG2	1.96	0.47
1:A:368:ILE:HD11	3:A:458:HOH:O	2.14	0.46
1:A:67:GLY:HA2	1:A:97:ASN:HD21	1.79	0.46
1:A:206:ASP:HB3	3:A:465:HOH:O	2.14	0.46
1:A:331:LYS:HB3	1:A:366:SER:HB2	1.97	0.46
1:A:289:THR:HG21	1:A:297:LEU:HD22	1.96	0.46
1:A:368:ILE:N	1:A:368:ILE:HD12	2.31	0.45
1:A:87:LEU:CD2	1:A:168[B]:CYS:SG	3.05	0.45
1:A:187:GLU:HG3	3:A:493:HOH:O	2.16	0.45
1:A:263:LEU:HD22	1:A:317:MSE:HE1	2.00	0.44
1:A:313:GLU:O	1:A:317:MSE:HB2	2.18	0.44
1:A:317:MSE:HE2	1:A:356:PRO:HG2	2.00	0.44
1:A:254:GLU:HG3	1:A:270:SER:HA	2.00	0.43
1:A:75:LYS:NZ	1:A:87:LEU:H	2.17	0.43
1:A:307:SER:HA	1:A:308:PRO:C	2.39	0.42
1:A:246:LYS:HA	1:A:247:PRO:HD3	1.90	0.42
1:A:248:MSE:HB2	1:A:278:CYS:SG	2.60	0.42
1:A:113:VAL:HG13	1:A:367:LEU:HB2	2.01	0.42
1:A:145:GLN:HB2	3:A:459:HOH:O	2.20	0.41
1:A:192:ILE:HD13	1:A:205:ILE:HD11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:GLY:HA2	1:A:309:PRO:O	2.19	0.41
1:A:277:THR:HG22	1:A:279:HIS:CE1	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:ARG:NH2	3:A:493:HOH:O[4_455]	2.12	0.08

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	307/368 (83%)	298 (97%)	9 (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	265/318 (83%)	264 (100%)	1 (0%)	93	92

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	328	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	ASN
1	A	223	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	DGI	A	369	-	23,29,29	1.11	2 (8%)	31,45,45	1.82	7 (22%)

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	DGI	A	369	-	-	0/12/28/28	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	369	DGI	C5-C4	2.88	1.47	1.40
2	A	369	DGI	C6-C5	3.43	1.48	1.41

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	369	DGI	C5-C6-N1	-4.00	118.12	123.59
2	A	369	DGI	C6-C5-C4	-3.74	116.43	120.90
2	A	369	DGI	N3-C2-N1	-3.45	122.18	127.44
2	A	369	DGI	C4-C5-N7	-3.03	106.69	109.48
2	A	369	DGI	C1'-N9-C4	-2.57	122.80	127.16
2	A	369	DGI	PA-O3A-PB	-2.07	125.73	132.67
2	A	369	DGI	C6-N1-C2	4.99	122.87	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	304/368 (82%)	2.44	148 (48%) 0 0	42, 54, 70, 73	4 (1%)

All (148) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	77	VAL	10.2
1	A	272	GLY	9.7
1	A	76	ILE	8.4
1	A	102	VAL	8.2
1	A	74	VAL	7.4
1	A	339	LEU	7.0
1	A	269	VAL	6.9
1	A	171	VAL	6.9
1	A	314	LEU	6.9
1	A	79	ILE	6.7
1	A	82	PHE	6.5
1	A	233	LYS	6.4
1	A	198	PRO	6.2
1	A	348	GLY	6.0
1	A	197	PHE	5.7
1	A	59[A]	PHE	5.6
1	A	320	LEU	5.4
1	A	346	GLU	5.3
1	A	166	VAL	5.3
1	A	101	LEU	5.3
1	A	340	GLY	5.3
1	A	297	LEU	5.2
1	A	87	LEU	5.2
1	A	73	VAL	5.2
1	A	176	PHE	5.2
1	A	347	PRO	5.1
1	A	251	GLN	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	367	LEU	5.0
1	A	57	ASP	5.0
1	A	85	SER	4.9
1	A	177	ILE	4.8
1	A	154	ILE	4.8
1	A	75	LYS	4.7
1	A	103	GLY	4.7
1	A	319	GLU	4.7
1	A	337	SER	4.7
1	A	338	GLY	4.7
1	A	86	TRP	4.6
1	A	326	ASN	4.6
1	A	336	PHE	4.5
1	A	315	GLU	4.5
1	A	329	GLU	4.4
1	A	72	LEU	4.4
1	A	165	VAL	4.3
1	A	207	ILE	4.3
1	A	61	ARG	4.3
1	A	168[A]	CYS	4.2
1	A	341	TRP	4.2
1	A	368	ILE	4.2
1	A	316	ASN	4.1
1	A	215	LEU	4.0
1	A	150	LEU	4.0
1	A	287	HIS	4.0
1	A	250	PHE	3.9
1	A	258	LEU	3.9
1	A	342	VAL	3.9
1	A	204	LEU	3.9
1	A	259	PHE	3.9
1	A	58	ASP	3.8
1	A	139	ILE	3.8
1	A	234	GLN	3.8
1	A	172	GLY	3.8
1	A	286	ILE	3.8
1	A	90	LEU	3.8
1	A	288	ARG	3.8
1	A	245	ILE	3.8
1	A	118	VAL	3.7
1	A	292	GLU	3.7
1	A	268	TYR	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	113	VAL	3.7
1	A	63	LEU	3.7
1	A	260	PHE	3.7
1	A	109	ILE	3.6
1	A	335	VAL	3.6
1	A	230	TYR	3.6
1	A	273	ARG	3.5
1	A	296	GLU	3.5
1	A	173	LYS	3.5
1	A	266	PHE	3.5
1	A	65	GLY	3.5
1	A	225	HIS	3.5
1	A	253	ASN	3.4
1	A	278	CYS	3.4
1	A	100	LEU	3.4
1	A	99	VAL	3.4
1	A	78	ASP	3.4
1	A	264	ALA	3.3
1	A	274	ARG	3.3
1	A	328	ARG	3.3
1	A	280	PHE	3.3
1	A	229	HIS	3.3
1	A	64	ASN	3.3
1	A	284	LEU	3.2
1	A	163	VAL	3.1
1	A	360	SER	3.1
1	A	205	ILE	3.0
1	A	167	GLY	3.0
1	A	80	PHE	3.0
1	A	84	GLY	3.0
1	A	353	ALA	2.8
1	A	112	SER	2.8
1	A	283	ARG	2.8
1	A	254	GLU	2.8
1	A	62	ILE	2.8
1	A	327	ILE	2.8
1	A	226	GLN	2.8
1	A	361	VAL	2.8
1	A	299	LYS	2.8
1	A	116	ASP	2.8
1	A	246	LYS	2.7
1	A	263	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	313	GLU	2.7
1	A	192	ILE	2.6
1	A	206	ASP	2.6
1	A	60	LEU	2.6
1	A	318	PRO	2.6
1	A	121	TRP	2.6
1	A	137	PHE	2.6
1	A	291	LEU	2.6
1	A	242	THR	2.6
1	A	304	ASP	2.6
1	A	104	ASN	2.5
1	A	56	ASP	2.5
1	A	257	THR	2.5
1	A	325	PHE	2.4
1	A	265	ARG	2.4
1	A	344	VAL	2.4
1	A	355	VAL	2.4
1	A	247	PRO	2.4
1	A	218	THR	2.4
1	A	186	ASP	2.4
1	A	209	LEU	2.3
1	A	276	PHE	2.3
1	A	216	TYR	2.3
1	A	349	ALA	2.3
1	A	359	VAL	2.3
1	A	131	LEU	2.2
1	A	305	LEU	2.2
1	A	221	ILE	2.2
1	A	184	PHE	2.1
1	A	66	ILE	2.1
1	A	306	LEU	2.1
1	A	255	GLU	2.1
1	A	232	GLY	2.1
1	A	147	ILE	2.1
1	A	138	LEU	2.0
1	A	270	SER	2.0
1	A	330	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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, 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	LLDF	B-factors(\AA^2)	Q<0.9
2	DGI	A	369	27/27	0.97	0.13	-1.10	34,39,42,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.