



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 09:23 PM GMT

PDB ID : 5A9Y
Title : Structure of ppGpp BipA
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Deposited on : 2015-07-23
Resolution : 4.00 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
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) : rb-20026982

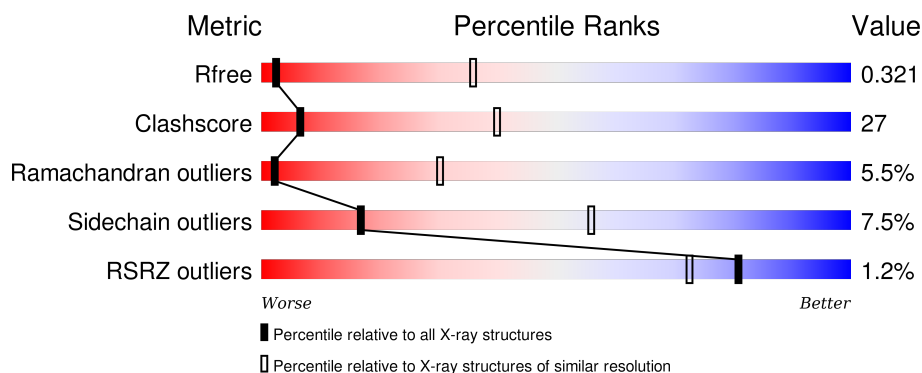
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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	1010 (4.42-3.56)
Clashscore	102246	1052 (4.40-3.60)
Ramachandran outliers	100387	1005 (4.40-3.60)
Sidechain outliers	100360	1013 (4.42-3.58)
RSRZ outliers	91569	1013 (4.42-3.56)

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	607	

2 Entry composition [i](#)

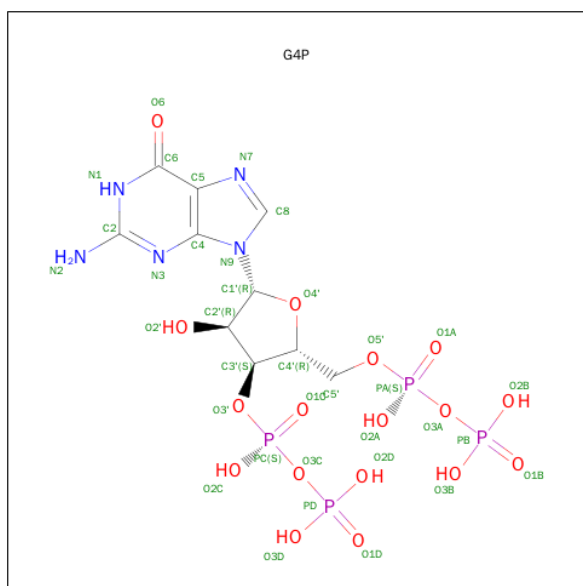
There are 3 unique types of molecules in this entry. The entry contains 4354 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	562	Total	C	N	O	S	0	0	0
			4301	2690	753	840	18			

- Molecule 2 is GUANOSINE-5',3'-TETRAPHOSPHATE (three-letter code: G4P) (formula: $C_{10}H_{17}N_5O_{17}P_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			36	10	5	17	4		

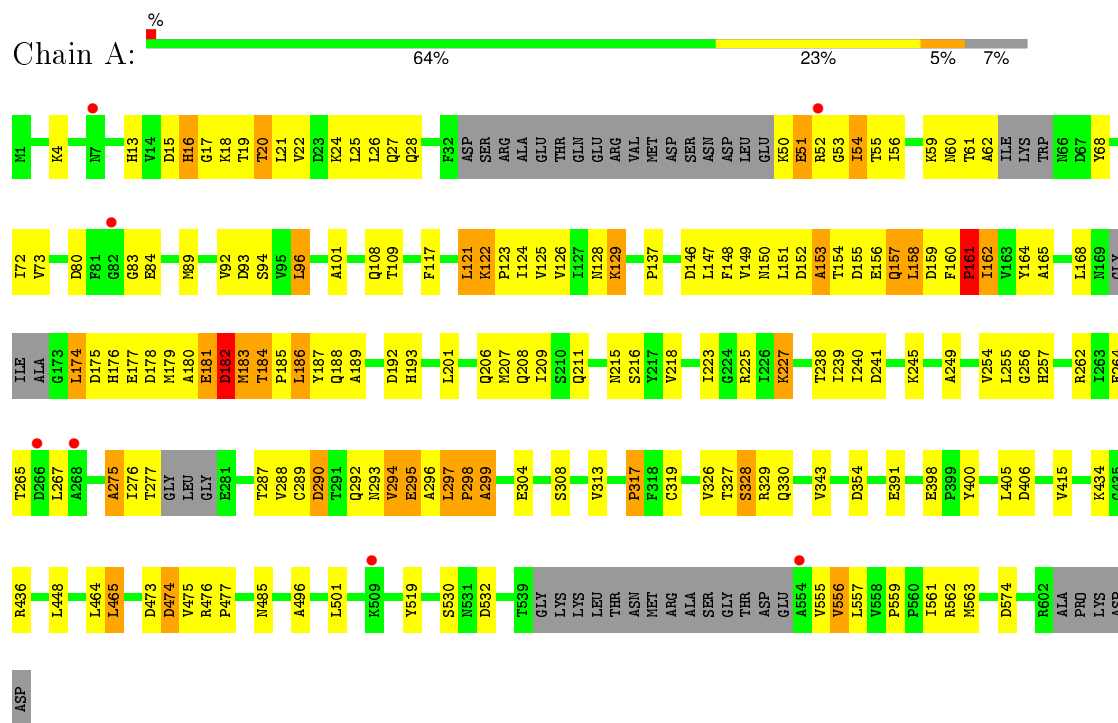
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	17	Total	0	0
			17		

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: GTP-BINDING PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	I 41 3 2	Depositor
Cell constants a, b, c, α , β , γ	244.31Å 244.31Å 244.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.91 – 4.00 47.91 – 4.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (47.91-4.00) 99.7 (47.91-4.00)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 4.00Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.254 , 0.321 0.272 , 0.321	Depositor DCC
R_{free} test set	809 reflections (8.11%)	DCC
Wilson B-factor (Å ²)	244.9	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 294.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 10783 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4354	wwPDB-VP
Average B, all atoms (Å ²)	293.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.86% 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: G4P

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	0.49	0/4361	0.67	4/5905 (0.1%)

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

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	161	PRO	N-CA-CB	5.93	110.41	103.30
1	A	559	PRO	C-N-CD	5.12	139.15	128.40
1	A	122	LYS	C-N-CD	5.06	139.03	128.40
1	A	297	LEU	C-N-CD	5.05	139.01	128.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	465	LEU	Peptide

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	4301	0	4237	234	0
2	A	36	0	11	5	0
3	A	17	0	0	1	0
All	All	4354	0	4248	234	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 27.

All (234) 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:94:SER:N	1:A:121:LEU:HD13	1.23	1.44
1:A:93:ASP:C	1:A:121:LEU:HD13	1.43	1.38
1:A:94:SER:CA	1:A:121:LEU:CD1	2.05	1.34
1:A:94:SER:CA	1:A:121:LEU:HD12	1.57	1.33
1:A:94:SER:N	1:A:121:LEU:CD1	2.02	1.21
1:A:94:SER:HA	1:A:121:LEU:CD1	1.66	1.15
1:A:178:ASP:HB2	1:A:179:MET:HB2	1.35	1.06
1:A:287:THR:HB	1:A:297:LEU:HD12	1.06	1.05
1:A:19:THR:HG21	1:A:22:VAL:HG23	1.35	1.03
1:A:55:THR:HG21	1:A:73:VAL:HG22	1.41	1.03
1:A:55:THR:HB	1:A:72:ILE:O	1.63	0.97
1:A:19:THR:HA	1:A:21:LEU:N	1.80	0.96
1:A:287:THR:HB	1:A:297:LEU:CD1	1.96	0.95
1:A:158:LEU:HA	1:A:159:ASP:HB3	1.49	0.94
1:A:94:SER:HA	1:A:121:LEU:HD12	0.94	0.94
1:A:181:GLU:O	1:A:183:MET:N	2.01	0.93
1:A:178:ASP:HB2	1:A:179:MET:CB	2.00	0.92
1:A:94:SER:CA	1:A:121:LEU:HD13	1.85	0.91
1:A:93:ASP:C	1:A:121:LEU:CD1	2.37	0.90
1:A:555:VAL:HA	1:A:556:VAL:HB	1.53	0.90
1:A:19:THR:HG21	1:A:22:VAL:CG2	2.04	0.88
1:A:177:GLU:HB3	1:A:178:ASP:HA	1.56	0.87
1:A:287:THR:CB	1:A:297:LEU:HD12	1.99	0.87
1:A:55:THR:CG2	1:A:73:VAL:HG22	2.05	0.87
1:A:19:THR:HA	1:A:21:LEU:H	1.34	0.85
1:A:555:VAL:HG13	1:A:557:LEU:HG	1.55	0.85
1:A:287:THR:HG21	1:A:297:LEU:CB	2.06	0.84
1:A:19:THR:CG2	1:A:22:VAL:HG23	2.08	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:THR:HB	1:A:22:VAL:N	1.93	0.83
1:A:240:ILE:HB	1:A:287:THR:OG1	1.80	0.82
1:A:294:VAL:HG12	1:A:295:GLU:H	1.44	0.81
1:A:158:LEU:HD12	1:A:193:HIS:HE1	1.45	0.81
1:A:16:HIS:O	2:A:1603:G4P:PA	2.39	0.80
1:A:239:ILE:CD1	1:A:288:VAL:CG2	2.60	0.80
1:A:156:GLU:HB3	1:A:159:ASP:HB2	1.63	0.79
1:A:147:LEU:O	1:A:150:ASN:OD1	2.00	0.79
1:A:94:SER:OG	1:A:122:LYS:O	2.00	0.78
1:A:555:VAL:CA	1:A:556:VAL:HB	2.14	0.77
1:A:153:ALA:HB3	1:A:154:THR:HA	1.65	0.77
1:A:164:TYR:OH	1:A:185:PRO:HG2	1.84	0.77
1:A:157:GLN:O	1:A:159:ASP:HB3	1.85	0.77
1:A:287:THR:HG21	1:A:297:LEU:HB3	1.66	0.76
1:A:19:THR:HB	1:A:22:VAL:H	1.47	0.76
1:A:239:ILE:HD12	1:A:288:VAL:CG2	2.16	0.76
1:A:160:PHE:CZ	1:A:162:ILE:HD12	2.22	0.75
1:A:160:PHE:CE1	1:A:162:ILE:HD12	2.22	0.75
1:A:19:THR:CA	1:A:20:THR:HB	2.16	0.75
1:A:16:HIS:C	2:A:1603:G4P:O1A	2.25	0.75
1:A:476:ARG:N	1:A:477:PRO:HA	2.01	0.75
1:A:239:ILE:HD12	1:A:288:VAL:HG21	1.68	0.74
1:A:55:THR:HG21	1:A:73:VAL:CG2	2.17	0.74
1:A:19:THR:HA	1:A:20:THR:HB	1.71	0.73
1:A:153:ALA:HB3	1:A:154:THR:CA	2.19	0.72
1:A:239:ILE:CD1	1:A:288:VAL:HG22	2.18	0.72
1:A:287:THR:HG21	1:A:297:LEU:HB2	1.69	0.72
1:A:239:ILE:HD13	1:A:288:VAL:HG22	1.71	0.72
1:A:93:ASP:O	1:A:121:LEU:CB	2.38	0.72
1:A:177:GLU:CB	1:A:178:ASP:HA	2.16	0.72
1:A:239:ILE:CD1	1:A:288:VAL:HG21	2.20	0.70
1:A:156:GLU:HA	1:A:157:GLN:C	2.12	0.70
1:A:156:GLU:HB3	1:A:159:ASP:CB	2.21	0.70
1:A:239:ILE:HD13	1:A:288:VAL:CG2	2.22	0.70
1:A:156:GLU:HB3	1:A:159:ASP:OD2	1.91	0.70
1:A:156:GLU:OE1	1:A:159:ASP:HB2	1.91	0.70
1:A:289:CYS:HB2	1:A:294:VAL:HG11	1.74	0.69
1:A:158:LEU:HD12	1:A:193:HIS:CE1	2.27	0.69
1:A:94:SER:C	1:A:121:LEU:HD12	2.12	0.69
1:A:555:VAL:CG1	1:A:557:LEU:HG	2.23	0.69
1:A:158:LEU:CB	1:A:160:PHE:HD1	2.04	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:ILE:HA	1:A:288:VAL:HG22	1.74	0.69
1:A:158:LEU:HB3	1:A:160:PHE:HD1	1.58	0.68
1:A:296:ALA:O	1:A:297:LEU:HD23	1.93	0.68
1:A:555:VAL:HA	1:A:556:VAL:O	1.93	0.68
1:A:158:LEU:HB3	1:A:160:PHE:CD1	2.29	0.68
1:A:94:SER:C	1:A:121:LEU:CD1	2.63	0.67
1:A:294:VAL:C	1:A:295:GLU:HG2	2.14	0.67
1:A:150:ASN:ND2	1:A:151:LEU:HD22	2.09	0.66
1:A:158:LEU:CA	1:A:159:ASP:HB3	2.24	0.66
1:A:19:THR:N	1:A:20:THR:HB	2.10	0.66
1:A:93:ASP:O	1:A:121:LEU:HB2	1.94	0.66
1:A:475:VAL:HG12	1:A:476:ARG:H	1.61	0.65
1:A:156:GLU:CB	1:A:159:ASP:HB2	2.26	0.64
1:A:164:TYR:OH	1:A:185:PRO:CG	2.46	0.63
1:A:177:GLU:HB3	1:A:178:ASP:CA	2.27	0.63
1:A:555:VAL:HA	1:A:556:VAL:CB	2.22	0.63
1:A:25:LEU:O	1:A:27:GLN:N	2.32	0.63
1:A:16:HIS:O	2:A:1603:G4P:O5'	2.16	0.63
1:A:240:ILE:HB	1:A:287:THR:HG1	1.62	0.62
1:A:25:LEU:O	1:A:27:GLN:HG3	2.00	0.61
1:A:51:GLU:HG2	1:A:52:ARG:HD3	1.82	0.61
1:A:475:VAL:HG12	1:A:477:PRO:HA	1.81	0.61
1:A:178:ASP:HB2	1:A:179:MET:CG	2.29	0.61
1:A:52:ARG:HB3	1:A:53:GLY:CA	2.31	0.61
1:A:160:PHE:HA	1:A:161:PRO:O	2.01	0.61
1:A:19:THR:CB	1:A:22:VAL:HB	2.32	0.60
1:A:55:THR:O	1:A:254:VAL:HG11	2.01	0.60
1:A:400:TYR:CE1	1:A:473:ASP:HB3	2.36	0.60
1:A:51:GLU:O	1:A:52:ARG:HD2	2.01	0.60
1:A:289:CYS:SG	1:A:294:VAL:HG11	2.43	0.59
1:A:186:LEU:O	1:A:187:TYR:C	2.41	0.59
1:A:128:ASN:HA	1:A:165:ALA:HB3	1.85	0.58
1:A:289:CYS:CB	1:A:294:VAL:HG11	2.33	0.58
1:A:19:THR:HB	1:A:22:VAL:HB	1.86	0.57
1:A:52:ARG:HB3	1:A:53:GLY:HA3	1.86	0.57
1:A:298:PRO:O	1:A:299:ALA:HB3	2.05	0.56
1:A:240:ILE:HD11	1:A:289:CYS:SG	2.45	0.56
1:A:240:ILE:HG21	1:A:296:ALA:HB1	1.86	0.56
1:A:158:LEU:HB2	1:A:160:PHE:HB2	1.88	0.56
1:A:158:LEU:CB	1:A:160:PHE:CD1	2.86	0.56
1:A:186:LEU:O	1:A:189:ALA:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:LEU:HA	1:A:159:ASP:CB	2.18	0.55
1:A:206:GLN:HG2	1:A:297:LEU:HD21	1.88	0.55
1:A:54:ILE:HG21	1:A:211:GLN:OE1	2.07	0.55
1:A:160:PHE:HA	1:A:161:PRO:C	2.26	0.55
1:A:238:THR:O	1:A:288:VAL:HG13	2.07	0.55
1:A:287:THR:CG2	1:A:297:LEU:HB2	2.37	0.54
1:A:156:GLU:HB3	1:A:159:ASP:CG	2.28	0.54
1:A:174:LEU:HD12	1:A:175:ASP:OD2	2.07	0.54
1:A:19:THR:CB	1:A:22:VAL:H	2.20	0.54
1:A:56:ILE:CD1	1:A:257:HIS:CE1	2.90	0.54
1:A:289:CYS:SG	1:A:294:VAL:CG1	2.96	0.54
1:A:160:PHE:CA	1:A:161:PRO:CB	2.86	0.53
1:A:292:GLN:O	1:A:294:VAL:HG23	2.08	0.53
1:A:164:TYR:CE1	1:A:182:ASP:CG	2.81	0.53
1:A:475:VAL:HB	1:A:477:PRO:HB3	1.91	0.53
1:A:294:VAL:HG12	1:A:295:GLU:N	2.21	0.52
1:A:155:ASP:HB2	1:A:156:GLU:OE2	2.10	0.52
1:A:158:LEU:CA	1:A:159:ASP:CB	2.86	0.52
1:A:56:ILE:HD13	1:A:257:HIS:CE1	2.44	0.52
1:A:153:ALA:N	1:A:154:THR:HA	2.24	0.52
1:A:180:ALA:O	1:A:182:ASP:N	2.42	0.52
1:A:16:HIS:O	2:A:1603:G4P:O1A	2.26	0.51
1:A:55:THR:HB	1:A:72:ILE:C	2.29	0.51
1:A:156:GLU:OE1	1:A:159:ASP:N	2.43	0.51
1:A:256:GLY:N	3:A:2005:HOH:O	2.44	0.51
1:A:153:ALA:CB	1:A:154:THR:HA	2.30	0.51
1:A:475:VAL:HG12	1:A:476:ARG:N	2.24	0.51
1:A:176:HIS:ND1	1:A:177:GLU:HA	2.25	0.51
1:A:13:HIS:HB3	1:A:109:THR:HG23	1.93	0.51
1:A:96:LEU:HD11	1:A:126:VAL:HG21	1.93	0.50
1:A:153:ALA:HB3	1:A:154:THR:C	2.31	0.50
1:A:89:MET:HA	1:A:92:VAL:HG22	1.94	0.50
1:A:53:GLY:C	1:A:54:ILE:HG12	2.32	0.50
1:A:84:GLU:HA	1:A:343:VAL:HG21	1.94	0.50
1:A:52:ARG:CB	1:A:53:GLY:CA	2.90	0.50
1:A:155:ASP:O	1:A:156:GLU:HG2	2.12	0.50
1:A:137:PRO:HG3	1:A:174:LEU:HD11	1.93	0.50
1:A:149:VAL:HG13	1:A:150:ASN:N	2.26	0.50
1:A:19:THR:HB	1:A:22:VAL:CB	2.41	0.49
1:A:18:LYS:C	1:A:20:THR:HB	2.32	0.49
1:A:287:THR:CB	1:A:297:LEU:HB2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:VAL:H	1:A:161:PRO:CB	2.26	0.49
1:A:287:THR:CG2	1:A:297:LEU:CB	2.86	0.49
1:A:555:VAL:HG13	1:A:557:LEU:CG	2.36	0.48
1:A:50:LYS:HE2	1:A:50:LYS:HA	1.95	0.48
1:A:123:PRO:O	1:A:124:ILE:HD13	2.13	0.48
1:A:19:THR:HA	1:A:20:THR:CB	2.37	0.48
1:A:184:THR:HA	1:A:187:TYR:CD2	2.48	0.48
1:A:17:GLY:N	2:A:1603:G4P:O1A	2.47	0.48
1:A:293:ASN:O	1:A:294:VAL:HG22	2.15	0.47
1:A:555:VAL:HG13	1:A:556:VAL:O	2.15	0.47
1:A:207:MET:HA	1:A:227:LYS:HG2	1.97	0.47
1:A:55:THR:O	1:A:254:VAL:CG1	2.62	0.47
1:A:146:ASP:O	1:A:149:VAL:HG12	2.15	0.47
1:A:209:ILE:HD12	1:A:209:ILE:N	2.30	0.46
1:A:93:ASP:O	1:A:121:LEU:HB3	2.14	0.46
1:A:55:THR:HG22	1:A:73:VAL:HA	1.98	0.46
1:A:164:TYR:CE1	1:A:182:ASP:OD1	2.68	0.46
1:A:295:GLU:HA	1:A:296:ALA:HA	1.61	0.46
1:A:158:LEU:HA	1:A:159:ASP:C	2.36	0.45
1:A:150:ASN:ND2	1:A:151:LEU:CD2	2.77	0.45
1:A:249:ALA:HB3	1:A:275:ALA:CB	2.46	0.45
1:A:555:VAL:CG1	1:A:557:LEU:CG	2.93	0.45
1:A:178:ASP:CB	1:A:179:MET:HB2	2.25	0.45
1:A:54:ILE:HG23	1:A:73:VAL:HG13	1.97	0.45
1:A:555:VAL:HA	1:A:556:VAL:C	2.35	0.45
1:A:326:VAL:C	1:A:330:GLN:HE22	2.20	0.45
1:A:276:ILE:HG22	1:A:277:THR:HG23	1.98	0.45
1:A:153:ALA:HB3	1:A:155:ASP:N	2.32	0.45
1:A:176:HIS:CG	1:A:177:GLU:HA	2.52	0.44
1:A:22:VAL:HA	1:A:25:LEU:HB2	1.99	0.44
1:A:101:ALA:HB2	1:A:128:ASN:O	2.17	0.44
1:A:178:ASP:CB	1:A:179:MET:CB	2.86	0.44
1:A:160:PHE:N	1:A:161:PRO:CB	2.81	0.44
1:A:19:THR:HA	1:A:20:THR:C	2.31	0.44
1:A:93:ASP:HA	1:A:121:LEU:HD22	1.99	0.44
1:A:293:ASN:C	1:A:294:VAL:CG2	2.86	0.44
1:A:176:HIS:O	1:A:179:MET:HE2	2.18	0.43
1:A:150:ASN:CG	1:A:151:LEU:HD22	2.38	0.43
1:A:327:THR:O	1:A:329:ARG:N	2.50	0.43
1:A:155:ASP:C	1:A:156:GLU:CG	2.86	0.43
1:A:160:PHE:HA	1:A:161:PRO:CB	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:TYR:OH	1:A:185:PRO:HB2	2.18	0.43
1:A:215:ASN:OD1	1:A:216:SER:N	2.51	0.43
1:A:177:GLU:CB	1:A:178:ASP:CA	2.93	0.43
1:A:150:ASN:HD21	1:A:151:LEU:CD2	2.32	0.43
1:A:317:PRO:HD2	1:A:519:TYR:CE1	2.54	0.43
1:A:61:THR:HG22	1:A:62:ALA:H	1.83	0.43
1:A:19:THR:OG1	1:A:22:VAL:HB	2.19	0.43
1:A:405:LEU:HD13	1:A:415:VAL:HG11	2.00	0.43
1:A:137:PRO:CG	1:A:174:LEU:HD11	2.48	0.43
1:A:208:GLN:HG3	1:A:287:THR:HG22	2.00	0.43
1:A:215:ASN:HB3	1:A:218:VAL:HB	1.99	0.43
1:A:149:VAL:CG1	1:A:150:ASN:N	2.81	0.43
1:A:93:ASP:O	1:A:121:LEU:HD13	2.05	0.43
1:A:183:MET:H	1:A:185:PRO:HD2	1.84	0.43
1:A:155:ASP:C	1:A:156:GLU:HG2	2.39	0.42
1:A:156:GLU:CA	1:A:157:GLN:CB	2.97	0.42
1:A:201:LEU:HA	1:A:267:LEU:HD22	2.01	0.42
1:A:117:PHE:HZ	1:A:148:PHE:CE1	2.37	0.42
1:A:313:VAL:HG21	1:A:328:SER:HB3	2.01	0.42
1:A:238:THR:HG23	1:A:245:LYS:HB3	2.01	0.42
1:A:485:ASN:HA	1:A:530:SER:HA	2.01	0.42
1:A:156:GLU:CD	1:A:156:GLU:N	2.73	0.42
1:A:56:ILE:HD11	1:A:257:HIS:CE1	2.54	0.42
1:A:555:VAL:N	1:A:556:VAL:HB	2.34	0.42
1:A:149:VAL:C	1:A:151:LEU:H	2.22	0.42
1:A:149:VAL:C	1:A:151:LEU:N	2.73	0.42
1:A:207:MET:SD	1:A:225:ARG:O	2.78	0.42
1:A:19:THR:CA	1:A:20:THR:CB	2.86	0.41
1:A:185:PRO:O	1:A:188:GLN:HB2	2.20	0.41
1:A:496:ALA:HB1	1:A:501:LEU:HD11	2.02	0.41
1:A:15:ASP:O	1:A:15:ASP:CG	2.58	0.41
1:A:287:THR:OG1	1:A:297:LEU:HB2	2.21	0.41
1:A:50:LYS:HA	1:A:51:GLU:HA	1.85	0.41
1:A:50:LYS:HB3	1:A:51:GLU:HB2	2.03	0.41
1:A:158:LEU:CD1	1:A:193:HIS:HE1	2.26	0.41
1:A:182:ASP:O	1:A:183:MET:SD	2.79	0.41
1:A:561:ILE:HG22	1:A:562:ARG:N	2.36	0.41
1:A:19:THR:HB	1:A:22:VAL:CA	2.52	0.41
1:A:53:GLY:O	1:A:54:ILE:HG12	2.21	0.40
1:A:238:THR:O	1:A:288:VAL:HA	2.21	0.40
1:A:182:ASP:O	1:A:183:MET:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:ASP:HB3	1:A:464:LEU:HB2	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	550/607 (91%)	418 (76%)	102 (18%)	30 (6%)	2 30

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	26	LEU
1	A	161	PRO
1	A	181	GLU
1	A	182	ASP
1	A	328	SER
1	A	80	ASP
1	A	129	LYS
1	A	223	ILE
1	A	241	ASP
1	A	290	ASP
1	A	294	VAL
1	A	298	PRO
1	A	434	LYS
1	A	51	GLU
1	A	152	ASP
1	A	153	ALA
1	A	168	LEU
1	A	16	HIS
1	A	20	THR
1	A	275	ALA

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Mol	Chain	Res	Type
1	A	183	MET
1	A	295	GLU
1	A	317	PRO
1	A	319	CYS
1	A	474	ASP
1	A	299	ALA
1	A	556	VAL
1	A	54	ILE
1	A	83	GLY
1	A	162	ILE

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	466 / 519 (90%)	431 (92%)	35 (8%)	17 56

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	24	LYS
1	A	28	GLN
1	A	59	LYS
1	A	60	ASN
1	A	68	TYR
1	A	96	LEU
1	A	108	GLN
1	A	121	LEU
1	A	129	LYS
1	A	157	GLN
1	A	158	LEU
1	A	174	LEU
1	A	182	ASP
1	A	184	THR
1	A	186	LEU

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Mol	Chain	Res	Type
1	A	192	ASP
1	A	227	LYS
1	A	255	LEU
1	A	262	ARG
1	A	264	GLU
1	A	265	THR
1	A	290	ASP
1	A	304	GLU
1	A	308	SER
1	A	354	ASP
1	A	391	GLU
1	A	398	GLU
1	A	436	ARG
1	A	448	LEU
1	A	465	LEU
1	A	474	ASP
1	A	532	ASP
1	A	563	MET
1	A	574	ASP

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

Mol	Chain	Res	Type
1	A	176	HIS
1	A	193	HIS
1	A	292	GLN
1	A	330	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

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	G4P	A	1603	-	30,38,38	1.17	2 (6%)	35,61,61	1.75	6 (17%)

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	G4P	A	1603	-	-	0/23/43/43	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1603	G4P	C5-C4	3.46	1.48	1.40
2	A	1603	G4P	C6-C5	4.07	1.49	1.41

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1603	G4P	C5-C6-N1	-4.58	117.53	123.52
2	A	1603	G4P	N3-C2-N1	-3.62	122.64	127.56
2	A	1603	G4P	C6-C5-C4	-2.57	117.92	120.86
2	A	1603	G4P	O3B-PB-O2B	2.07	115.03	107.44
2	A	1603	G4P	C3'-C2'-C1'	2.35	105.17	100.06
2	A	1603	G4P	C6-N1-C2	5.75	122.62	115.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1603	G4P	5	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	562/607 (92%)	0.03	7 (1%)	81 72	208, 291, 364, 443	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	52	ARG	2.8
1	A	509	LYS	2.7
1	A	7	ASN	2.3
1	A	554	ALA	2.3
1	A	268	ALA	2.3
1	A	266	ASP	2.3
1	A	82	GLY	2.1

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, 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	G4P	A	1603	36/36	0.74	0.23	-0.58	260,341,500,500	0

6.5 Other polymers [i](#)

There are no such residues in this entry.