



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 06:57 PM GMT

PDB ID : 4JVS  
Title : Crystal structure of LepB GAP domain from Legionella drancourtii in complex with Rab1-GDP and AIF3  
Authors : Yu, Q.; Yao, Q.; Wang, D.-C.; Shao, F.  
Deposited on : 2013-03-26  
Resolution : 2.78 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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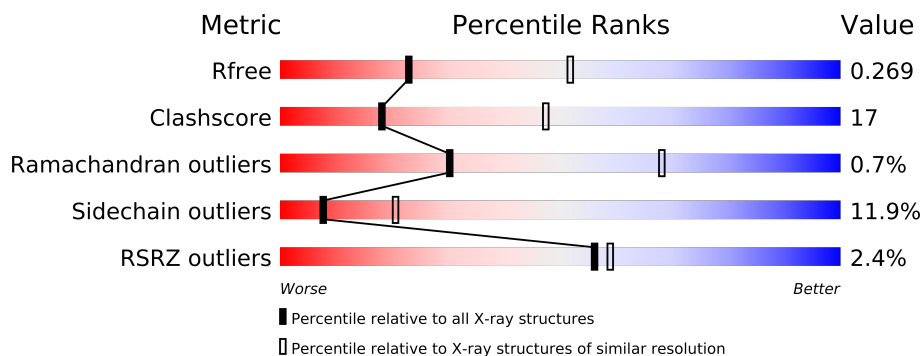
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.78 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))
$R_{free}$	66092	2193 (2.80-2.76)
Clashscore	79885	2751 (2.80-2.76)
Ramachandran outliers	78287	2699 (2.80-2.76)
Sidechain outliers	78261	2701 (2.80-2.76)
RSRZ outliers	66119	2196 (2.80-2.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	310	
2	B	181	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
6	MG	B	402	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 3655 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	279	2252	1422	391	425	14	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	311	SER	-	EXPRESSION TAG	UNP G9EPL4
A	312	GLY	-	EXPRESSION TAG	UNP G9EPL4
A	313	ARG	-	EXPRESSION TAG	UNP G9EPL4
A	314	PRO	-	EXPRESSION TAG	UNP G9EPL4
A	315	MET	-	EXPRESSION TAG	UNP G9EPL4

- Molecule 2 is a protein called Ras-related protein Rab-1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	170	1362	868	222	267	5	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

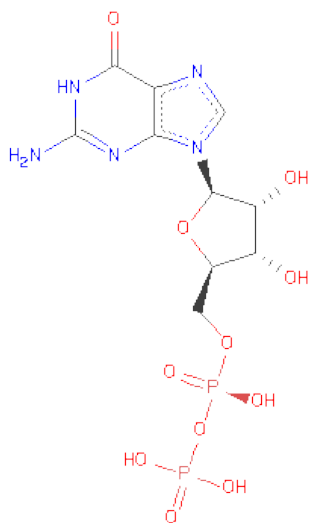
Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	SER	-	EXPRESSION TAG	UNP P62820
B	-2	GLY	-	EXPRESSION TAG	UNP P62820
B	-1	ARG	-	EXPRESSION TAG	UNP P62820
B	0	PRO	-	EXPRESSION TAG	UNP P62820

- Molecule 3 is ACETIC ACID (three-letter code: ACY) (formula: C<sub>2</sub>H<sub>4</sub>O<sub>2</sub>).



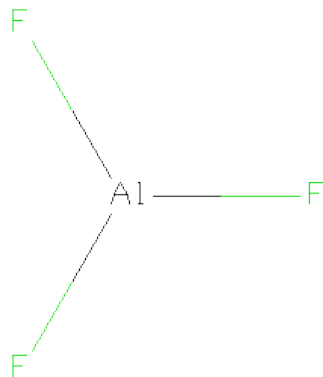
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 5 is ALUMINUM FLUORIDE (three-letter code: AF3) (formula:  $AlF_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	Al	F	0	0
			4	1	3		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Mg	0	0
			1	1		

- Molecule 7 is water.

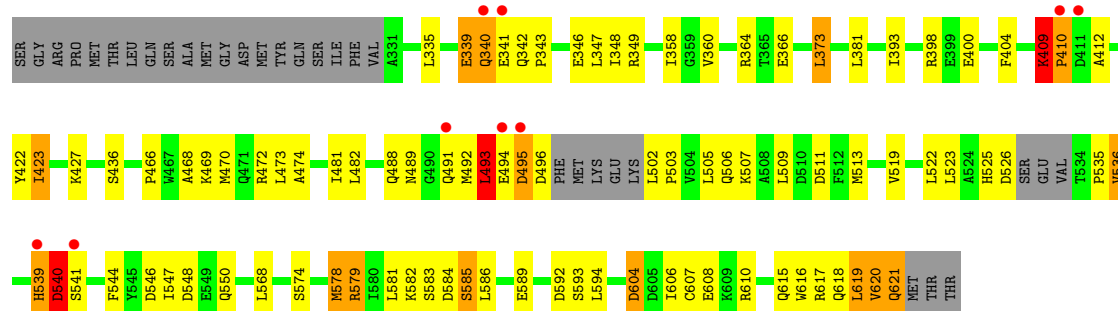
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	O	0	0
			1	1		
7	B	3	Total	O	0	0
			3	3		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

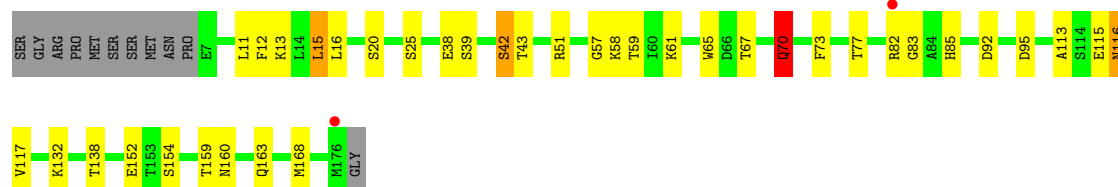
- Molecule 1: Putative uncharacterized protein

Chain A: 



- Molecule 2: Ras-related protein Rab-1A

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	95.56Å 95.56Å 197.72Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.96 – 2.78 19.96 – 2.78	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.96-2.78) 99.6 (19.96-2.78)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.39 (at 2.79Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1069)	Depositor
R, $R_{free}$	0.224 , 0.265 0.226 , 0.269	Depositor DCC
$R_{free}$ test set	701 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	40.1	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 16.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 13979 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	3655	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, ACY, MG, AF3

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	0.86	0/2304	0.75	4/3122 (0.1%)
2	B	0.59	0/1384	0.65	2/1868 (0.1%)
All	All	0.77	0/3688	0.72	6/4990 (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	3

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	409	LYS	C-N-CD	-9.66	99.34	120.60
2	B	70	GLN	OE1-CD-NE2	-7.51	104.63	121.90
2	B	70	GLN	CG-CD-NE2	7.22	134.03	116.70
1	A	540	ASP	CB-CG-OD1	-6.93	112.07	118.30
1	A	493	LEU	CA-CB-CG	6.05	129.21	115.30
1	A	540	ASP	CB-CG-OD2	5.04	122.83	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	409	LYS	Peptide
1	A	489	ASN	Peptide

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Mol	Chain	Res	Type	Group
1	A	540	ASP	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2252	0	2168	100	2
2	B	1362	0	1357	19	0
3	A	4	0	3	11	0
4	B	28	0	12	5	0
5	B	4	0	0	3	0
6	B	1	0	0	0	0
7	A	1	0	0	0	0
7	B	3	0	0	0	0
All	All	3655	0	3540	122	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 17.

All (122) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:547:ILE:O	1:A:579:ARG:NH1	1.59	1.35
1:A:579:ARG:NH2	3:A:701:ACY:O	1.60	1.34
1:A:547:ILE:H	3:A:701:ACY:CH3	1.64	1.10
1:A:616:TRP:O	1:A:620:VAL:HG22	1.50	1.09
1:A:346:GLU:OE2	1:A:349:ARG:NH1	1.92	1.02
1:A:494:GLU:HA	1:A:495:ASP:HB3	1.42	1.00
1:A:494:GLU:HG3	1:A:495:ASP:O	1.67	0.95
1:A:493:LEU:C	1:A:494:GLU:OE1	2.09	0.91
1:A:427:LYS:NZ	1:A:539:HIS:ND1	2.19	0.91
1:A:493:LEU:O	1:A:494:GLU:OE1	1.89	0.91
1:A:494:GLU:HA	1:A:495:ASP:CB	1.98	0.90
1:A:539:HIS:NE2	1:A:544:PHE:O	2.07	0.87
2:B:38:GLU:OE2	4:B:400:GDP:O2'	1.92	0.87
1:A:341:GLU:O	1:A:341:GLU:HG3	1.76	0.84

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:616:TRP:O	1:A:620:VAL:CG2	2.25	0.83
1:A:547:ILE:H	3:A:701:ACY:H1	1.43	0.82
1:A:546:ASP:HA	3:A:701:ACY:H1	1.61	0.82
1:A:547:ILE:N	3:A:701:ACY:CH3	2.41	0.81
1:A:495:ASP:N	1:A:496:ASP:HB2	1.95	0.81
1:A:494:GLU:CB	1:A:495:ASP:O	2.30	0.80
1:A:494:GLU:CG	1:A:495:ASP:O	2.30	0.79
2:B:160:ASN:HA	2:B:163:GLN:OE1	1.82	0.79
1:A:594:LEU:HD22	1:A:610:ARG:HG3	1.68	0.75
1:A:340:GLN:HG3	1:A:341:GLU:N	2.00	0.74
1:A:488:GLN:HG3	1:A:488:GLN:O	1.90	0.71
1:A:502:LEU:HG	1:A:502:LEU:O	1.92	0.69
1:A:494:GLU:CA	1:A:495:ASP:O	2.41	0.68
4:B:400:GDP:H5"	4:B:400:GDP:H8	1.57	0.68
1:A:427:LYS:NZ	1:A:539:HIS:CE1	2.62	0.67
1:A:548:ASP:C	1:A:548:ASP:OD1	2.30	0.67
1:A:502:LEU:N	1:A:503:PRO:HD2	2.09	0.67
1:A:583:SER:HB3	1:A:586:LEU:HB2	1.76	0.67
1:A:539:HIS:CD2	1:A:541:SER:H	2.12	0.66
1:A:547:ILE:H	3:A:701:ACY:H3	1.59	0.65
1:A:493:LEU:O	1:A:494:GLU:CD	2.35	0.65
1:A:495:ASP:H	1:A:496:ASP:HB2	1.58	0.65
1:A:583:SER:O	1:A:585:SER:N	2.29	0.65
1:A:493:LEU:HD22	1:A:493:LEU:H	1.63	0.64
1:A:495:ASP:CA	1:A:496:ASP:HB2	2.28	0.64
1:A:502:LEU:O	1:A:506:GLN:HG3	1.97	0.64
1:A:339:GLU:HB2	1:A:342:GLN:HG3	1.79	0.64
1:A:339:GLU:CB	1:A:342:GLN:HG3	2.27	0.63
1:A:339:GLU:HB2	1:A:342:GLN:CG	2.28	0.63
2:B:15:LEU:HD22	2:B:65:TRP:HB2	1.79	0.63
1:A:427:LYS:HZ1	1:A:539:HIS:CE1	2.13	0.62
1:A:539:HIS:CE1	1:A:544:PHE:O	2.53	0.62
1:A:491:GLN:O	1:A:492:MET:HG3	1.99	0.62
2:B:42:SER:OG	5:B:401:AF3:F3	2.07	0.60
1:A:494:GLU:CA	1:A:495:ASP:CB	2.76	0.60
2:B:113:ALA:HB1	2:B:117:VAL:HG21	1.84	0.60
1:A:540:ASP:N	1:A:540:ASP:OD1	2.30	0.60
4:B:400:GDP:PB	5:B:401:AF3:F2	2.50	0.59
1:A:340:GLN:HG3	1:A:341:GLU:H	1.66	0.59
4:B:400:GDP:H5"	4:B:400:GDP:C8	2.37	0.59
1:A:540:ASP:O	1:A:541:SER:OG	2.22	0.57
1:A:525:HIS:ND1	1:A:525:HIS:C	2.56	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:539:HIS:C	1:A:540:ASP:OD1	2.43	0.57
1:A:502:LEU:N	1:A:503:PRO:CD	2.65	0.57
1:A:578:MET:O	1:A:582:LYS:HB2	2.06	0.55
1:A:335:LEU:HB2	1:A:364:ARG:NH2	2.21	0.55
1:A:493:LEU:H	1:A:493:LEU:CD2	2.18	0.54
1:A:427:LYS:HE3	1:A:539:HIS:CE1	2.43	0.54
1:A:547:ILE:N	3:A:701:ACY:H1	2.16	0.54
1:A:615:GLN:O	1:A:618:GLN:HG2	2.08	0.54
2:B:159:THR:O	2:B:160:ASN:HB2	2.07	0.53
1:A:539:HIS:HD2	1:A:546:ASP:OD1	1.92	0.52
2:B:116:ASN:OD1	2:B:116:ASN:N	2.42	0.52
1:A:604:ASP:OD1	1:A:604:ASP:N	2.30	0.51
1:A:617:ARG:O	1:A:620:VAL:HG23	2.10	0.51
1:A:469:LYS:HD2	1:A:522:LEU:HD11	1.91	0.51
1:A:348:ILE:HG23	1:A:509:LEU:HD22	1.92	0.51
1:A:617:ARG:O	1:A:621:GLN:HG2	2.11	0.51
2:B:154:SER:HB3	2:B:159:THR:HB	1.93	0.51
1:A:546:ASP:HA	3:A:701:ACY:CH3	2.37	0.51
1:A:525:HIS:ND1	1:A:526:ASP:N	2.58	0.51
1:A:540:ASP:O	3:A:701:ACY:OXT	2.28	0.50
1:A:473:LEU:HD22	1:A:519:VAL:HG21	1.92	0.50
1:A:548:ASP:OD1	1:A:548:ASP:O	2.29	0.50
1:A:373:LEU:HD13	1:A:481:ILE:HG12	1.93	0.50
1:A:410:PRO:HA	1:A:412:ALA:N	2.26	0.50
1:A:507:LYS:NZ	1:A:511:ASP:OD2	2.44	0.50
2:B:92:ASP:HB3	2:B:95:ASP:HB3	1.92	0.50
2:B:25:SER:OG	4:B:400:GDP:O2B	2.22	0.49
1:A:492:MET:O	1:A:493:LEU:O	2.30	0.49
1:A:436:SER:HB3	1:A:474:ALA:HB1	1.95	0.49
1:A:618:GLN:HG3	1:A:619:LEU:N	2.28	0.48
2:B:11:LEU:HD23	2:B:61:LYS:HB3	1.95	0.48
1:A:427:LYS:CE	1:A:539:HIS:CE1	2.97	0.48
2:B:20:SER:HA	5:B:401:AF3:F1	2.04	0.47
1:A:494:GLU:HB3	1:A:495:ASP:O	2.12	0.47
1:A:494:GLU:HA	1:A:495:ASP:O	2.14	0.47
2:B:70:GLN:HG2	2:B:73:PHE:HD2	1.79	0.46
1:A:468:ALA:O	1:A:472:ARG:HB2	2.16	0.46
1:A:409:LYS:HD3	1:A:422:TYR:CD2	2.51	0.46
1:A:536:VAL:H	1:A:536:VAL:HG13	1.37	0.45
1:A:539:HIS:NE2	1:A:541:SER:N	2.63	0.44
1:A:621:GLN:HG3	1:A:621:GLN:H	1.39	0.44
1:A:606:ILE:HA	1:A:606:ILE:HD12	1.74	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:341:GLU:O	1:A:341:GLU:CG	2.56	0.44
1:A:539:HIS:CG	1:A:540:ASP:N	2.86	0.44
1:A:547:ILE:N	3:A:701:ACY:H2	2.30	0.44
1:A:522:LEU:HD23	1:A:522:LEU:HA	1.63	0.44
1:A:536:VAL:O	1:A:536:VAL:CG2	2.63	0.43
2:B:58:LYS:HD2	2:B:58:LYS:N	2.33	0.43
1:A:423:ILE:HG21	1:A:544:PHE:CE1	2.53	0.43
1:A:539:HIS:CD2	1:A:540:ASP:N	2.87	0.43
1:A:583:SER:OG	1:A:583:SER:O	2.29	0.43
1:A:494:GLU:N	1:A:494:GLU:OE1	2.50	0.43
1:A:339:GLU:HG3	1:A:342:GLN:HB2	2.01	0.43
1:A:342:GLN:HA	1:A:343:PRO:HD3	1.65	0.43
2:B:57:GLY:C	2:B:58:LYS:HD2	2.39	0.43
1:A:339:GLU:HG2	1:A:347:LEU:HD13	2.01	0.42
1:A:618:GLN:CG	1:A:619:LEU:N	2.83	0.42
1:A:579:ARG:NH2	3:A:701:ACY:C	2.64	0.42
1:A:493:LEU:CD2	1:A:493:LEU:N	2.82	0.42
2:B:12:PHE:HA	2:B:85:HIS:ND1	2.35	0.41
1:A:502:LEU:HB3	1:A:503:PRO:HD3	2.02	0.41
1:A:466:PRO:O	1:A:470:MET:HG2	2.20	0.41
1:A:608:GLU:OE1	1:A:608:GLU:N	2.48	0.41
2:B:13:LYS:HD2	2:B:83:GLY:O	2.21	0.41
2:B:132:LYS:NZ	2:B:152:GLU:OE2	2.49	0.40
2:B:67:THR:HB	2:B:77:THR:HG21	2.02	0.40

All (2) 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	Distance(Å)	Clash(Å)
1:A:607:CYS:SG	1:A:607:CYS:SG[10_555]	1.35	0.85
1:A:398:ARG:NH2	1:A:592:ASP:OD2[6_554]	2.19	0.01

## 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	273/310 (88%)	260 (95%)	10 (4%)	3 (1%)	21	55
2	B	168/181 (93%)	163 (97%)	5 (3%)	0	100	100
All	All	441/491 (90%)	423 (96%)	15 (3%)	3 (1%)	30	68

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	410	PRO
1	A	493	LEU
1	A	495	ASP

### 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	245/274 (89%)	211 (86%)	34 (14%)	5	14
2	B	150/159 (94%)	137 (91%)	13 (9%)	15	37
All	All	395/433 (91%)	348 (88%)	47 (12%)	8	20

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	339	GLU
1	A	340	GLN
1	A	358	ILE
1	A	360	VAL
1	A	366	GLU
1	A	373	LEU
1	A	381	LEU
1	A	393	ILE
1	A	400	GLU
1	A	404	PHE
1	A	409	LYS
1	A	423	ILE
1	A	482	LEU
1	A	493	LEU

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Mol	Chain	Res	Type
1	A	505	LEU
1	A	513	MET
1	A	523	LEU
1	A	535	PRO
1	A	536	VAL
1	A	539	HIS
1	A	550	GLN
1	A	568	LEU
1	A	574	SER
1	A	578	MET
1	A	579	ARG
1	A	581	LEU
1	A	584	ASP
1	A	585	SER
1	A	589	GLU
1	A	593	SER
1	A	604	ASP
1	A	619	LEU
1	A	620	VAL
1	A	621	GLN
2	B	15	LEU
2	B	16	LEU
2	B	39	SER
2	B	42	SER
2	B	43	THR
2	B	51	ARG
2	B	59	THR
2	B	70	GLN
2	B	82	ARG
2	B	115	GLU
2	B	116	ASN
2	B	138	THR
2	B	168	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	618	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 for Mogul analysis.

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$
3	ACY	A	701	-	3,3,3	0.87	0	3,3,3	0.62	0
4	GDP	B	400	6	30,30,30	2.51	6 (20%)	44,47,47	2.23	13 (29%)
5	AF3	B	401	-	0,3,3	0.00	-	0,3,3	0.00	-

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
3	ACY	A	701	-	-	0/0/0/0	0/0/0/0
4	GDP	B	400	6	-	0/16/32/32	0/1/3/3
5	AF3	B	401	-	-	0/0/0/0	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	400	GDP	C4-N3	7.83	1.48	1.35
4	B	400	GDP	C2-N2	7.59	1.44	1.32
4	B	400	GDP	C2-N1	3.85	1.42	1.36
4	B	400	GDP	C6-C5	3.11	1.46	1.41
4	B	400	GDP	C2'-C1'	-2.40	1.50	1.53
4	B	400	GDP	C4-N9	2.25	1.41	1.37

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	400	GDP	C6-C5-N7	-7.49	133.13	134.14
4	B	400	GDP	N3-C4-N9	4.55	133.58	126.91
4	B	400	GDP	C5-C4-N3	-4.43	119.53	125.94
4	B	400	GDP	C2-N3-C4	4.28	121.10	115.09
4	B	400	GDP	O4'-C1'-N9	3.96	112.12	108.44
4	B	400	GDP	C5'-C4'-C3'	-3.62	100.70	115.21
4	B	400	GDP	N2-C2-N1	3.40	121.60	117.86
4	B	400	GDP	PA-O3A-PB	-2.99	122.92	131.68
4	B	400	GDP	C6-N1-C2	2.80	124.40	119.51
4	B	400	GDP	N1-C2-N3	-2.65	118.06	121.78
4	B	400	GDP	C4-C5-N7	-2.17	107.66	109.52
4	B	400	GDP	C8-N9-C4	-2.10	105.29	106.90
4	B	400	GDP	C3'-C2'-C1'	2.02	104.07	100.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	279/310 (90%)	-0.03	9 (3%) 45 48	24, 45, 65, 85	0
2	B	170/181 (93%)	-0.12	2 (1%) 75 78	32, 46, 63, 76	0
All	All	449/491 (91%)	-0.06	11 (2%) 56 59	24, 45, 64, 85	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	411	ASP	4.9
1	A	340	GLN	4.2
1	A	495	ASP	4.0
1	A	539	HIS	3.6
1	A	410	PRO	3.1
2	B	82	ARG	2.9
1	A	341	GLU	2.4
1	A	541	SER	2.3
1	A	491	GLN	2.2
2	B	176	MET	2.1
1	A	494	GLU	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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	MG	B	402	1/1	0.21	2.01	36,36,36,36	0
5	AF3	B	401	4/4	0.18	1.34	34,34,35,35	0
4	GDP	B	400	28/28	0.16	0.48	29,38,43,48	0
3	ACY	A	701	4/4	0.15	-0.87	48,49,52,53	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.