W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 06:32 PM GMT

PDB ID	:	4LWZ
Title	:	Crystal structure of Myo5b globular tail domain in complex with inactive Rab11a
Authors	:	Pylypenko, O.; Attanda, W.; Gauquelin, C.; Houdusse, A.
Deposited on	:	2013-07-29
Resolution	:	2.55 Å(reported)

The following versions of software and data (see references (i)) 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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	Percentile Ranks	Value
Rfree		0.287
Clashscore		5
Ramachandran outliers		0.1%
Sidechain outliers		3.1%
RSRZ outliers		11.1%

Worse　　　　　　　　　　　　　　　　　*Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
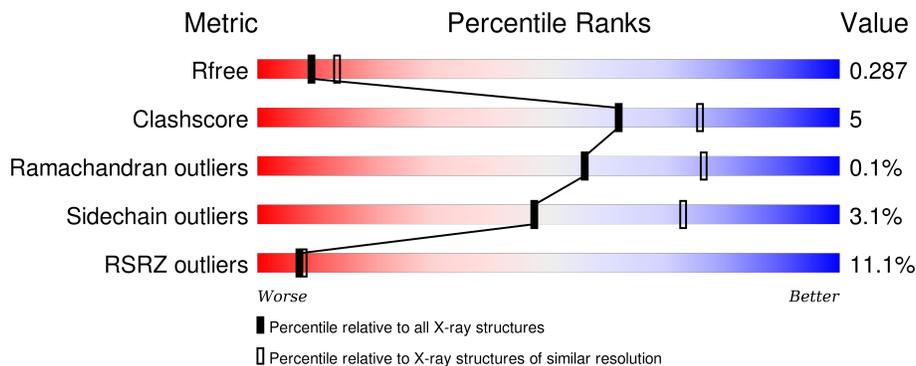
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	4549 (2.58-2.50)
Clashscore	102246	5292 (2.58-2.50)
Ramachandran outliers	100387	5194 (2.58-2.50)
Sidechain outliers	100360	5196 (2.58-2.50)
RSRZ outliers	91569	4561 (2.58-2.50)

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 <=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	177	8%　80%　11%　•　8%
1	C	177	15%　71%　15%　•　12%
2	B	427	4%　79%　6%　14%
2	D	427	13%　68%　13%　19%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8137 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 Ras-related protein Rab-11A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	162	Total 1265	C 803	N 215	O 246	S 1	0	0	0
1	C	155	Total 1174	C 739	N 206	O 228	S 1	0	0	0

- Molecule 2 is a protein called Unconventional myosin-Vb.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	367	Total 2903	C 1847	N 492	O 539	S 25	0	1	0
2	D	346	Total 2612	C 1651	N 447	O 493	S 21	0	0	0

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1422	MET	-	EXPRESSION TAG	UNP Q9ULV0
B	1423	ARG	-	EXPRESSION TAG	UNP Q9ULV0
B	1424	SER	-	EXPRESSION TAG	UNP Q9ULV0
B	1425	GLU	-	EXPRESSION TAG	UNP Q9ULV0
B	1426	THR	-	EXPRESSION TAG	UNP Q9ULV0
B	1427	MET	-	EXPRESSION TAG	UNP Q9ULV0
B	1428	SER	-	EXPRESSION TAG	UNP Q9ULV0
B	1429	TYR	-	EXPRESSION TAG	UNP Q9ULV0
B	1430	TYR	-	EXPRESSION TAG	UNP Q9ULV0
B	1431	HIS	-	EXPRESSION TAG	UNP Q9ULV0
B	1432	HIS	-	EXPRESSION TAG	UNP Q9ULV0
B	1433	HIS	-	EXPRESSION TAG	UNP Q9ULV0
B	1434	HIS	-	EXPRESSION TAG	UNP Q9ULV0
B	1435	HIS	-	EXPRESSION TAG	UNP Q9ULV0
B	1436	HIS	-	EXPRESSION TAG	UNP Q9ULV0
B	1437	ASP	-	EXPRESSION TAG	UNP Q9ULV0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1438	TYR	-	EXPRESSION TAG	UNP Q9ULV0
B	1439	ASP	-	EXPRESSION TAG	UNP Q9ULV0
B	1440	ILE	-	EXPRESSION TAG	UNP Q9ULV0
B	1441	PRO	-	EXPRESSION TAG	UNP Q9ULV0
B	1442	THR	-	EXPRESSION TAG	UNP Q9ULV0
B	1443	THR	-	EXPRESSION TAG	UNP Q9ULV0
B	1444	GLU	-	EXPRESSION TAG	UNP Q9ULV0
B	1445	ASN	-	EXPRESSION TAG	UNP Q9ULV0
B	1446	LEU	-	EXPRESSION TAG	UNP Q9ULV0
B	1447	TYR	-	EXPRESSION TAG	UNP Q9ULV0
B	1448	PHE	-	EXPRESSION TAG	UNP Q9ULV0
B	1449	GLN	-	EXPRESSION TAG	UNP Q9ULV0
B	1450	GLY	-	EXPRESSION TAG	UNP Q9ULV0
B	1451	ALA	-	EXPRESSION TAG	UNP Q9ULV0
B	1452	MET	-	EXPRESSION TAG	UNP Q9ULV0
B	1453	GLY	-	EXPRESSION TAG	UNP Q9ULV0
B	1454	SER	-	EXPRESSION TAG	UNP Q9ULV0
B	1455	MET	-	EXPRESSION TAG	UNP Q9ULV0
D	1422	MET	-	EXPRESSION TAG	UNP Q9ULV0
D	1423	ARG	-	EXPRESSION TAG	UNP Q9ULV0
D	1424	SER	-	EXPRESSION TAG	UNP Q9ULV0
D	1425	GLU	-	EXPRESSION TAG	UNP Q9ULV0
D	1426	THR	-	EXPRESSION TAG	UNP Q9ULV0
D	1427	MET	-	EXPRESSION TAG	UNP Q9ULV0
D	1428	SER	-	EXPRESSION TAG	UNP Q9ULV0
D	1429	TYR	-	EXPRESSION TAG	UNP Q9ULV0
D	1430	TYR	-	EXPRESSION TAG	UNP Q9ULV0
D	1431	HIS	-	EXPRESSION TAG	UNP Q9ULV0
D	1432	HIS	-	EXPRESSION TAG	UNP Q9ULV0
D	1433	HIS	-	EXPRESSION TAG	UNP Q9ULV0
D	1434	HIS	-	EXPRESSION TAG	UNP Q9ULV0
D	1435	HIS	-	EXPRESSION TAG	UNP Q9ULV0
D	1436	HIS	-	EXPRESSION TAG	UNP Q9ULV0
D	1437	ASP	-	EXPRESSION TAG	UNP Q9ULV0
D	1438	TYR	-	EXPRESSION TAG	UNP Q9ULV0
D	1439	ASP	-	EXPRESSION TAG	UNP Q9ULV0
D	1440	ILE	-	EXPRESSION TAG	UNP Q9ULV0
D	1441	PRO	-	EXPRESSION TAG	UNP Q9ULV0
D	1442	THR	-	EXPRESSION TAG	UNP Q9ULV0
D	1443	THR	-	EXPRESSION TAG	UNP Q9ULV0
D	1444	GLU	-	EXPRESSION TAG	UNP Q9ULV0
D	1445	ASN	-	EXPRESSION TAG	UNP Q9ULV0

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1446	LEU	-	EXPRESSION TAG	UNP Q9ULV0
D	1447	TYR	-	EXPRESSION TAG	UNP Q9ULV0
D	1448	PHE	-	EXPRESSION TAG	UNP Q9ULV0
D	1449	GLN	-	EXPRESSION TAG	UNP Q9ULV0
D	1450	GLY	-	EXPRESSION TAG	UNP Q9ULV0
D	1451	ALA	-	EXPRESSION TAG	UNP Q9ULV0
D	1452	MET	-	EXPRESSION TAG	UNP Q9ULV0
D	1453	GLY	-	EXPRESSION TAG	UNP Q9ULV0
D	1454	SER	-	EXPRESSION TAG	UNP Q9ULV0
D	1455	MET	-	EXPRESSION TAG	UNP Q9ULV0

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).
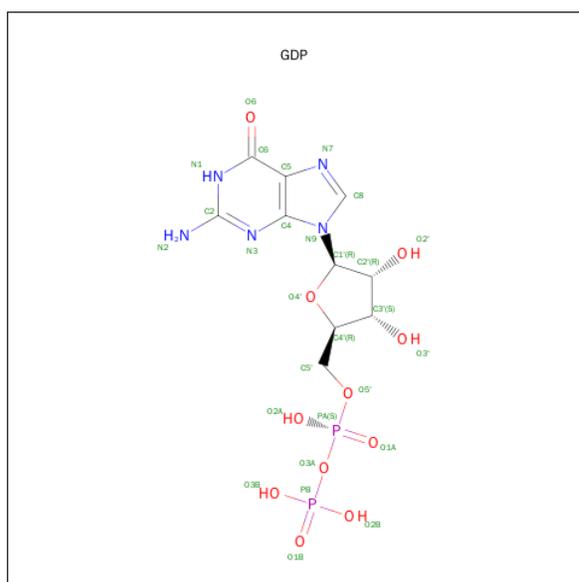
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
3	C	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total 1	Mg 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	33	Total 33	O 33	0	0
5	B	49	Total 49	O 49	0	0
5	C	17	Total 17	O 17	0	0
5	D	26	Total 26	O 26	0	0

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: Ras-related protein Rab-11A
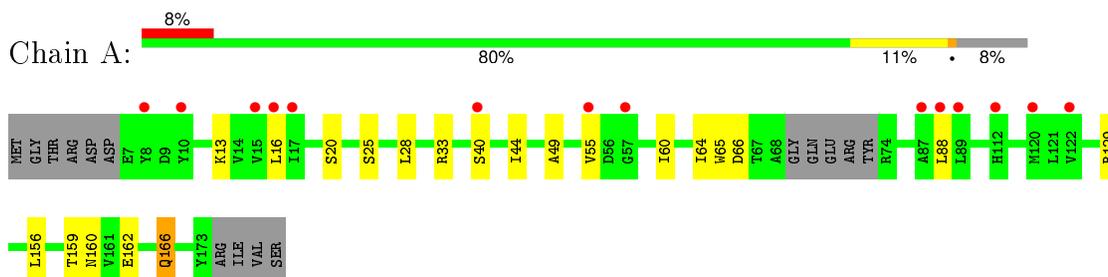
- Molecule 1: Ras-related protein Rab-11A
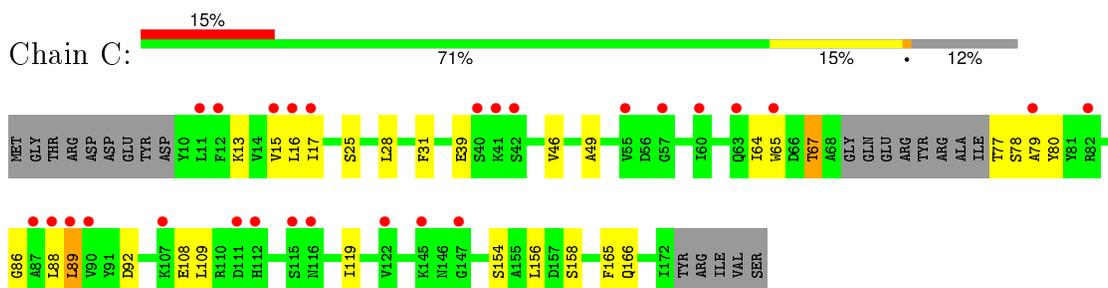
- Molecule 2: Unconventional myosin-Vb
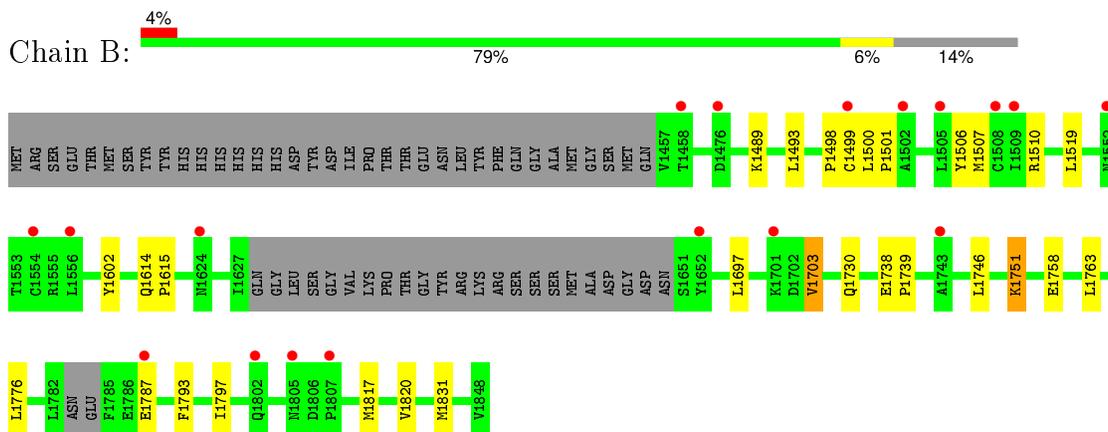
- Molecule 2: Unconventional myosin-Vb
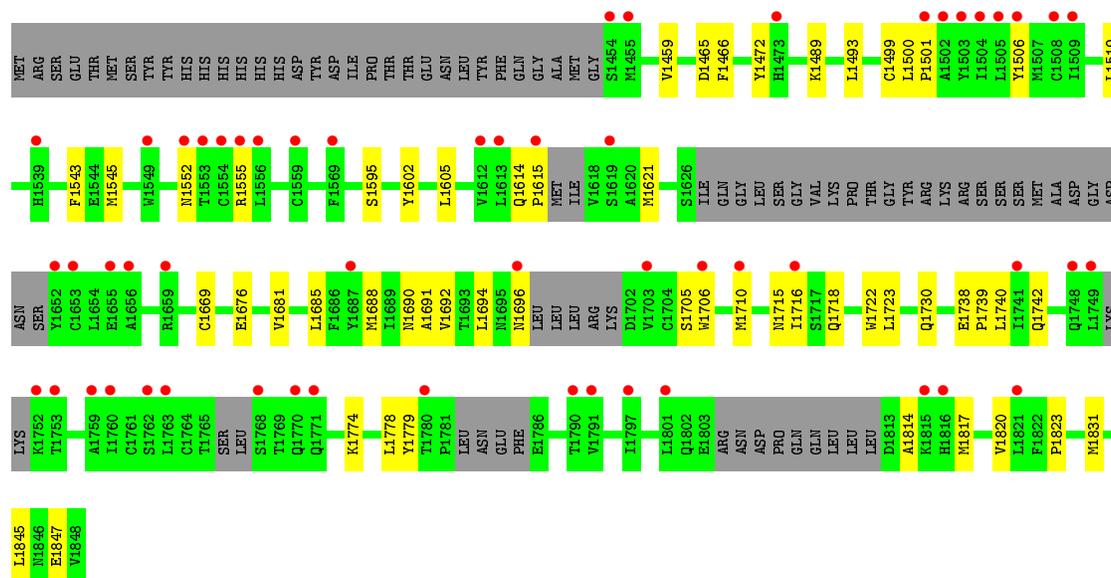
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	67.68Å 143.14Å 162.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.97 – 2.55 24.97 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.7 (24.97-2.55) 99.7 (24.97-2.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.61 (at 2.54Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.231 , 0.295 0.222 , 0.287	Depositor DCC
R_{free} test set	2605 reflections (5.00%)	DCC
Wilson B-factor (Å^2)	66.8	Xtriage
Anisotropy	0.689	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 60.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Outliers	0 of 52116 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8137	wwPDB-VP
Average B, all atoms (Å^2)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: GDP, MG

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	0.39	0/1285	0.54	0/1742
1	C	0.40	0/1191	0.55	0/1614
2	B	0.38	0/2955	0.49	0/4000
2	D	0.38	0/2653	0.51	0/3598
All	All	0.39	0/8084	0.51	0/10954

There are no bond length outliers.

There are no bond angle outliers.

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	1265	0	1236	15	0
1	C	1174	0	1123	24	0
2	B	2903	0	2882	17	0
2	D	2612	0	2435	31	0
3	A	28	0	12	1	0
3	C	28	0	12	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	A	33	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	49	0	0	0	0
5	C	17	0	0	0	0
5	D	26	0	0	0	0
All	All	8137	0	7700	85	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 5.

The worst 5 of 85 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)
2:D:1602:TYR:CZ	2:D:1820:VAL:HG11	2.19	0.78
2:B:1602:TYR:CZ	2:B:1820:VAL:HG11	2.26	0.71
2:B:1507:MET:HG3	2:B:1831:MET:CE	2.25	0.67
1:C:13:LYS:HE3	1:C:65:TRP:CE2	2.32	0.64
2:D:1602:TYR:CE2	2:D:1820:VAL:HG11	2.33	0.63

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	158/177 (89%)	153 (97%)	5 (3%)	0	100	100
1	C	151/177 (85%)	141 (93%)	10 (7%)	0	100	100
2	B	362/427 (85%)	345 (95%)	17 (5%)	0	100	100
2	D	330/427 (77%)	312 (94%)	17 (5%)	1 (0%)	46	66
All	All	1001/1208 (83%)	951 (95%)	49 (5%)	1 (0%)	56	76

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	1694	LEU

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	132/150 (88%)	129 (98%)	3 (2%)	58	82
1	C	118/150 (79%)	112 (95%)	6 (5%)	29	50
2	B	321/391 (82%)	312 (97%)	9 (3%)	51	76
2	D	266/391 (68%)	258 (97%)	8 (3%)	48	74
All	All	837/1082 (77%)	811 (97%)	26 (3%)	47	73

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	1817	MET
1	C	39	GLU
2	D	1730	GLN
1	C	17	ILE
1	C	25	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	1511	HIS
2	B	1539	HIS
2	D	1539	HIS

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)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	GDP	A	201	4	23,30,30	1.18	2 (8%)	30,47,47	2.17	9 (30%)
3	GDP	C	201	4	23,30,30	1.14	3 (13%)	30,47,47	2.08	8 (26%)

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	GDP	A	201	4	-	0/12/32/32	0/3/3/3
3	GDP	C	201	4	-	0/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	201	GDP	C5-C4	2.24	1.45	1.40
3	C	201	GDP	O4'-C1'	2.55	1.44	1.41
3	C	201	GDP	C5-C4	2.57	1.46	1.40
3	C	201	GDP	C6-C5	3.30	1.47	1.41
3	A	201	GDP	C6-C5	3.55	1.48	1.41

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	201	GDP	C2'-C1'-N9	-4.60	107.27	114.29
3	A	201	GDP	C5-C6-N1	-4.45	117.50	123.59
3	C	201	GDP	C6-C5-C4	-4.13	115.96	120.90
3	C	201	GDP	C5-C6-N1	-3.90	118.25	123.59
3	A	201	GDP	C1'-N9-C4	-3.89	121.07	126.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	201	GDP	1	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	162/177 (91%)	0.23	14 (8%)	13	14	52, 77, 128, 162	0
1	C	155/177 (87%)	0.83	27 (17%)	2	2	60, 97, 141, 181	0
2	B	367/427 (85%)	0.11	18 (4%)	33	39	54, 81, 140, 188	0
2	D	346/427 (81%)	0.56	55 (15%)	3	3	59, 98, 146, 178	0
All	All	1030/1208 (85%)	0.39	114 (11%)	7	8	52, 90, 142, 188	0

The worst 5 of 114 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	1652	TYR	6.6
2	B	1624	ASN	6.0
2	D	1710	MET	5.9
1	C	55	VAL	5.8
2	D	1760	ILE	5.7

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(Å^2)	Q<0.9
4	MG	A	202	1/1	0.97	0.11	-0.77	74,74,74,74	0
3	GDP	A	201	28/28	0.98	0.11	-1.08	47,61,72,83	0
3	GDP	C	201	28/28	0.96	0.13	-1.22	56,70,84,96	0
4	MG	C	202	1/1	0.70	0.17	-	90,90,90,90	0

6.5 Other polymers (i)

There are no such residues in this entry.