wwPDB X-ray Structure Validation Summary Report (i)

Sep 13, 2020 – 02:26 PM BST

PDB ID	:	4BL6
Title	:	Bicaudal-D uses a parallel, homodimeric coiled coil with heterotypic registry to co-ordinate recruitment of cargos to dynein
Authors	:	Liu, Y.; Salter, H.K.; Holding, A.N.; Johnson, C.M.; Stephens, E.; Lukavsky, P.J.; Walshaw, J.; Bullock, S.L.
Deposited on	:	2013-05-02
Resolution	:	2.18 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

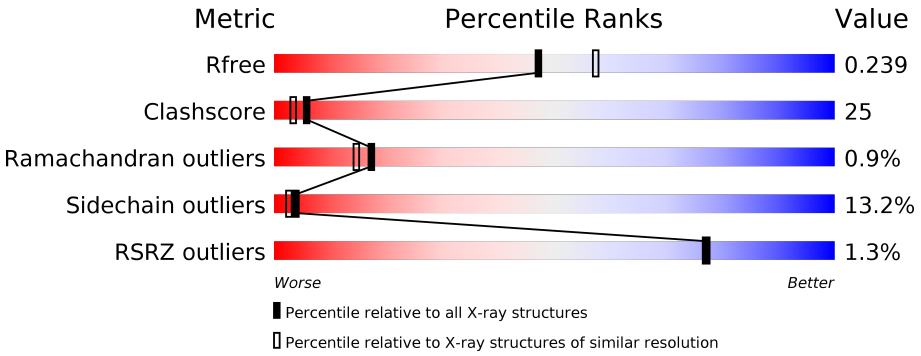
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.4.dev1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.4.dev1

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 2.18 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}	130704	6864 (2.20-2.16)
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)
RSRZ outliers	127900	6738 (2.20-2.16)

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 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 <=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	94	51% 28% 7% • 13%
1	B	94	49% 26% 5% 20%
1	C	94	3% 59% 27% 5% • 9%
1	D	94	% 51% 32% 5% • 11%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2678 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.

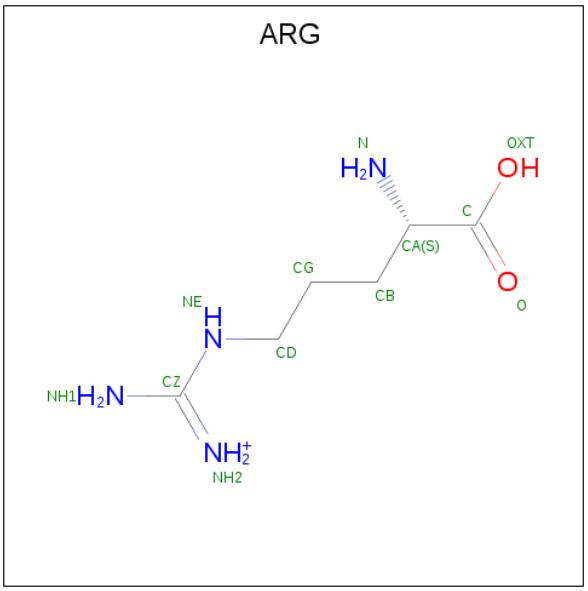
- Molecule 1 is a protein called PROTEIN BICAUDAL D.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	82	Total	C	N	O	S	Se	0	0	0
			643	400	110	128	1	4			
1	B	75	Total	C	N	O	S	Se	0	0	0
			599	370	109	117	1	2			
1	C	86	Total	C	N	O	S	Se	0	0	0
			656	407	118	128	1	2			
1	D	84	Total	C	N	O	S	Se	0	0	0
			670	413	121	132	1	3			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	652	GLY	-	expression tag	UNP P16568
A	653	SER	-	expression tag	UNP P16568
A	654	HIS	-	expression tag	UNP P16568
A	655	MSE	-	expression tag	UNP P16568
B	652	GLY	-	expression tag	UNP P16568
B	653	SER	-	expression tag	UNP P16568
B	654	HIS	-	expression tag	UNP P16568
B	655	MSE	-	expression tag	UNP P16568
C	652	GLY	-	expression tag	UNP P16568
C	653	SER	-	expression tag	UNP P16568
C	654	HIS	-	expression tag	UNP P16568
C	655	MSE	-	expression tag	UNP P16568
D	652	GLY	-	expression tag	UNP P16568
D	653	SER	-	expression tag	UNP P16568
D	654	HIS	-	expression tag	UNP P16568
D	655	MSE	-	expression tag	UNP P16568

- Molecule 2 is ARGININE (three-letter code: ARG) (formula: $C_6H_{15}N_4O_2$).



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

- Molecule 3 is water.

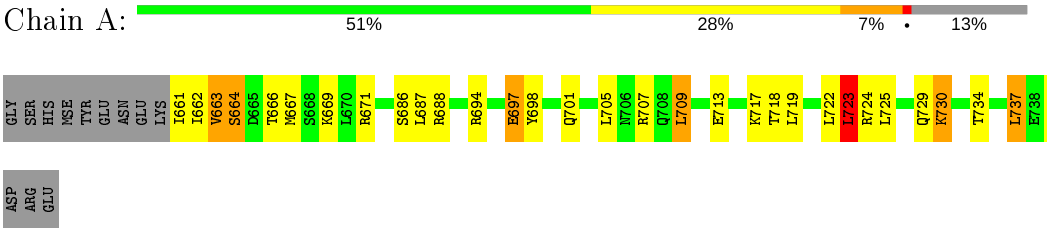
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	23	Total O 23 23	0	0
3	B	27	Total O 27 27	0	0
3	C	22	Total O 22 22	0	0
3	D	34	Total O 34 34	0	0

3 Residue-property plots (i)

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.

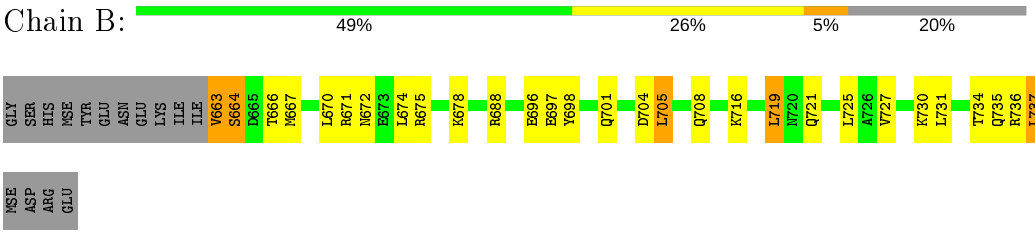
- Molecule 1: PROTEIN BICAUDAL D

Chain A:



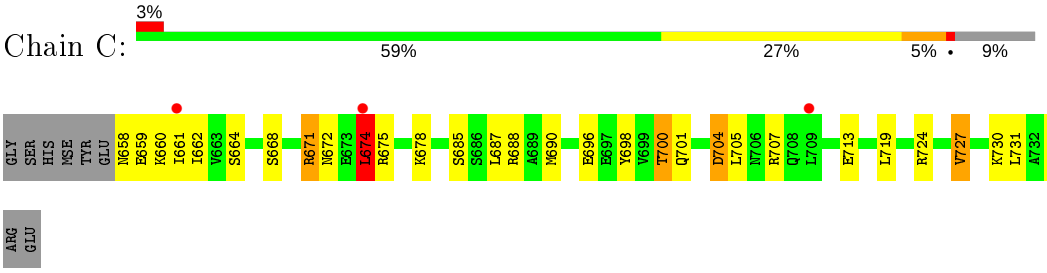
- Molecule 1: PROTEIN BICAUDAL D

Chain B:



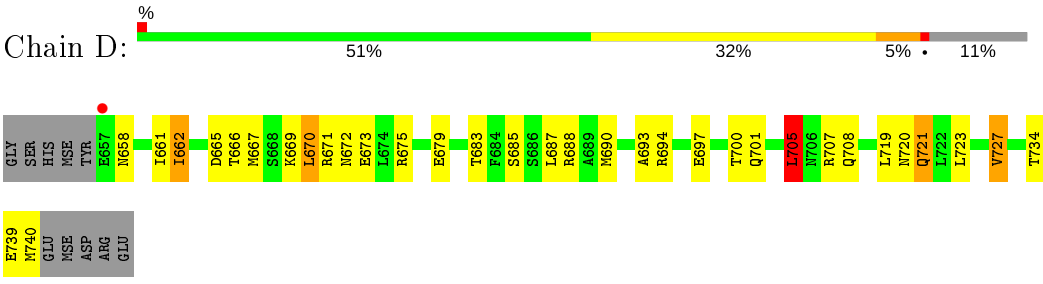
- Molecule 1: PROTEIN BICAUDAL D

Chain C:



- Molecule 1: PROTEIN BICAUDAL D

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	62.20Å 62.20Å 190.51Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.89 – 2.18 46.89 – 2.18	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.89-2.18) 100.0 (46.89-2.18)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.51 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.204 , 0.235 0.205 , 0.239	Depositor DCC
R_{free} test set	1749 reflections (8.02%)	wwPDB-VP
Wilson B-factor (Å^2)	33.8	Xtriage
Anisotropy	0.513	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 22.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.468 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.523 for H, K, L 0.477 for -H-K, K, -L	Depositor
Outliers	0 of 21820 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	2678	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.65% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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	1.29	2/641 (0.3%)	1.30	4/854 (0.5%)
1	B	1.35	0/599	1.23	2/801 (0.2%)
1	C	1.28	2/654 (0.3%)	1.23	4/873 (0.5%)
1	D	1.13	0/669	1.18	4/891 (0.4%)
All	All	1.26	4/2563 (0.2%)	1.23	14/3419 (0.4%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	698	TYR	CD2-CE2	-6.25	1.29	1.39
1	A	697	GLU	CD-OE2	5.85	1.32	1.25
1	C	713	GLU	CG-CD	5.43	1.60	1.51
1	C	713	GLU	CB-CG	5.37	1.62	1.52

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	674	LEU	CA-CB-CG	8.23	134.24	115.30
1	C	707	ARG	NE-CZ-NH2	-7.61	116.50	120.30
1	D	665	ASP	CB-CG-OD1	7.09	124.69	118.30
1	D	670	LEU	CB-CG-CD1	-7.04	99.04	111.00
1	A	723	LEU	CA-CB-CG	6.08	129.28	115.30

There are no chirality outliers.

There are no planarity outliers.

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	643	0	651	39	0
1	B	599	0	614	46	0
1	C	656	0	650	31	0
1	D	670	0	682	40	0
2	C	4	0	1	0	0
3	A	23	0	0	2	0
3	B	27	0	0	4	0
3	C	22	0	0	0	0
3	D	34	0	0	10	0
All	All	2678	0	2598	131	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 25.

The worst 5 of 131 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:737:LEU:O	1:A:741:GLU:HB3	1.52	1.07
1:D:675:ARG:HD3	3:D:808:HOH:O	1.56	1.06
1:B:664:SER:OG	1:B:666:THR:HG22	1.56	1.05
1:B:671:ARG:NH1	1:B:674:LEU:HD23	1.72	1.02
1:A:671:ARG:HH22	1:B:719:LEU:CD1	1.80	0.94

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	80/94 (85%)	76 (95%)	2 (2%)	2 (2%)	5 2
1	B	73/94 (78%)	70 (96%)	2 (3%)	1 (1%)	11 8
1	C	84/94 (89%)	79 (94%)	5 (6%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	82/94 (87%)	78 (95%)	4 (5%)	0	100 100
All	All	319/376 (85%)	303 (95%)	13 (4%)	3 (1%)	17 15

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	664	SER
1	A	663	VAL
1	A	664	SER

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	69/79 (87%)	62 (90%)	7 (10%)	7 6
1	B	65/79 (82%)	60 (92%)	5 (8%)	13 12
1	C	66/79 (84%)	55 (83%)	11 (17%)	2 1
1	D	72/79 (91%)	59 (82%)	13 (18%)	1 1
All	All	272/316 (86%)	236 (87%)	36 (13%)	4 2

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	687	LEU
1	C	719	LEU
1	D	727	VAL
1	C	700	THR
1	C	727	VAL

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

Mol	Chain	Res	Type
1	B	701	GLN

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Mol	Chain	Res	Type
1	B	708	GLN
1	D	720	ASN

5.3.3 RNA

There are no RNA molecules 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 monosaccharides 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	ARG	C	801	-	2,3,11	0.09	0	1,3,13	0.49	0

There are no bond length outliers.

There are no bond angle outliers.

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, 95^{th} 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	78/94 (82%)	0.17	0	100	100	19, 32, 54, 79	0
1	B	73/94 (77%)	0.06	0	100	100	23, 31, 49, 62	0
1	C	82/94 (87%)	0.15	3 (3%)	41	42	23, 36, 56, 63	0
1	D	81/94 (86%)	0.25	1 (1%)	79	79	27, 38, 57, 72	0
All	All	314/376 (83%)	0.16	4 (1%)	77	77	19, 35, 57, 79	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	709	LEU	2.5
1	C	674	LEU	2.4
1	D	657	GLU	2.3
1	C	661	ILE	2.3

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 monosaccharides 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. The B-factors column lists the minimum, median, 95^{th} 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	B-factors(Å^2)	Q<0.9
2	ARG	C	801	4/12	0.89	0.22	63,63,63,63	0

6.5 Other polymers (i)

There are no such residues in this entry.