wwPDB X-ray Structure Validation Summary Report (i)

Jun 16, 2024 – 07:29 AM EDT

PDB ID	:	5CEA
Title	:	Bd3460 Immunity Protein from Bdellovibrio bacteriovorus
Authors	:	Lovering, A.L.; Cadby, I.T.; Lambert, C.; Sockett, R.E.
Deposited on	:	2015-07-06
Resolution	:	1.85 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

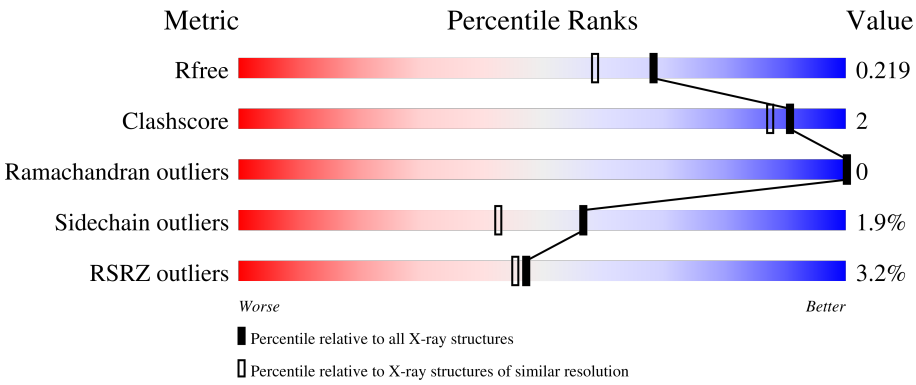
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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 of 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	230	79% 5% 16%
1	B	230	78% 6% • 15%
1	C	230	81% • • 15%
1	D	230	5% 80% • 16%
1	E	230	8% 77% 5% 17%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7800 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 Bd3460.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	193	1430	890	248	288	4	0	0	0
1	D	193	1441	898	250	289	4	0	2	0
1	C	196	1459	910	253	292	4	0	1	0
1	B	195	1448	902	252	290	4	0	0	0
1	E	190	1411	879	244	284	4	0	0	0

There are 55 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	MET	ALA	engineered mutation	UNP Q6MHS9
A	221	LEU	-	expression tag	UNP Q6MHS9
A	222	GLU	-	expression tag	UNP Q6MHS9
A	223	HIS	-	expression tag	UNP Q6MHS9
A	224	HIS	-	expression tag	UNP Q6MHS9
A	225	HIS	-	expression tag	UNP Q6MHS9
A	226	HIS	-	expression tag	UNP Q6MHS9
A	227	HIS	-	expression tag	UNP Q6MHS9
A	228	HIS	-	expression tag	UNP Q6MHS9
A	229	HIS	-	expression tag	UNP Q6MHS9
A	230	HIS	-	expression tag	UNP Q6MHS9
D	25	MET	ALA	engineered mutation	UNP Q6MHS9
D	221	LEU	-	expression tag	UNP Q6MHS9
D	222	GLU	-	expression tag	UNP Q6MHS9
D	223	HIS	-	expression tag	UNP Q6MHS9
D	224	HIS	-	expression tag	UNP Q6MHS9
D	225	HIS	-	expression tag	UNP Q6MHS9
D	226	HIS	-	expression tag	UNP Q6MHS9
D	227	HIS	-	expression tag	UNP Q6MHS9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	228	HIS	-	expression tag	UNP Q6MHS9
D	229	HIS	-	expression tag	UNP Q6MHS9
D	230	HIS	-	expression tag	UNP Q6MHS9
C	25	MET	ALA	engineered mutation	UNP Q6MHS9
C	221	LEU	-	expression tag	UNP Q6MHS9
C	222	GLU	-	expression tag	UNP Q6MHS9
C	223	HIS	-	expression tag	UNP Q6MHS9
C	224	HIS	-	expression tag	UNP Q6MHS9
C	225	HIS	-	expression tag	UNP Q6MHS9
C	226	HIS	-	expression tag	UNP Q6MHS9
C	227	HIS	-	expression tag	UNP Q6MHS9
C	228	HIS	-	expression tag	UNP Q6MHS9
C	229	HIS	-	expression tag	UNP Q6MHS9
C	230	HIS	-	expression tag	UNP Q6MHS9
B	25	MET	ALA	engineered mutation	UNP Q6MHS9
B	221	LEU	-	expression tag	UNP Q6MHS9
B	222	GLU	-	expression tag	UNP Q6MHS9
B	223	HIS	-	expression tag	UNP Q6MHS9
B	224	HIS	-	expression tag	UNP Q6MHS9
B	225	HIS	-	expression tag	UNP Q6MHS9
B	226	HIS	-	expression tag	UNP Q6MHS9
B	227	HIS	-	expression tag	UNP Q6MHS9
B	228	HIS	-	expression tag	UNP Q6MHS9
B	229	HIS	-	expression tag	UNP Q6MHS9
B	230	HIS	-	expression tag	UNP Q6MHS9
E	25	MET	ALA	engineered mutation	UNP Q6MHS9
E	221	LEU	-	expression tag	UNP Q6MHS9
E	222	GLU	-	expression tag	UNP Q6MHS9
E	223	HIS	-	expression tag	UNP Q6MHS9
E	224	HIS	-	expression tag	UNP Q6MHS9
E	225	HIS	-	expression tag	UNP Q6MHS9
E	226	HIS	-	expression tag	UNP Q6MHS9
E	227	HIS	-	expression tag	UNP Q6MHS9
E	228	HIS	-	expression tag	UNP Q6MHS9
E	229	HIS	-	expression tag	UNP Q6MHS9
E	230	HIS	-	expression tag	UNP Q6MHS9

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	152	152	152	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	98	Total O 98 98	0	0
2	C	159	Total O 159 159	0	0
2	B	171	Total O 171 171	0	0
2	E	31	Total O 31 31	0	0

3 Residue-property plots (i)

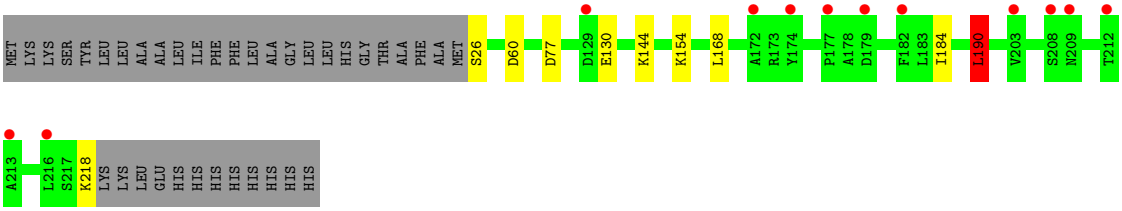
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Bd3460

Chain A:

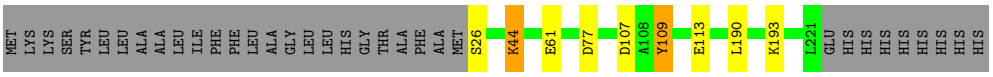
- Molecule 1: Bd3460

Chain D:



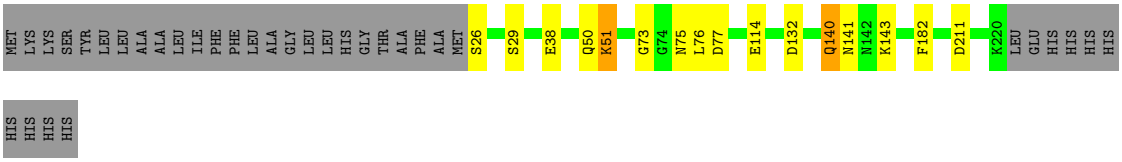
- Molecule 1: Bd3460

Chain C:



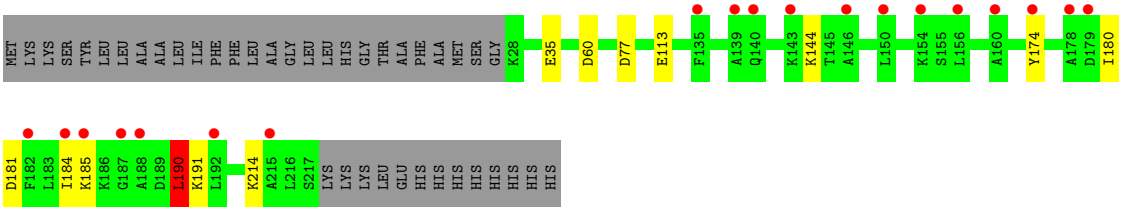
- Molecule 1: Bd3460

Chain B:



- Molecule 1: Bd3460

Chain E:


MET LYS LYS SER TYR LEU LEU ALA ALA LEU ILE PHE PHE LEU ALA GLY LEU LEU HIS GLY THR ALA PHE ALA MET SER GLY K28 E35 D60 D77 E113 F135 A139 Q140 K143 K144 T145 A146 L150 K154 S155 L156 A160 Y174 A178 D179 I180
D181 F182 L183 I184 K185 K186 G187 A188 D189 L190 K191 L192 K214 A215 L216 S217 LYS LYS LYS LEU GLU HIS HIS HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	57.43Å 99.64Å 173.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	86.85 – 1.85 50.06 – 1.85	Depositor EDS
% Data completeness (in resolution range)	98.7 (86.85-1.85) 98.7 (50.06-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.20 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.176 , 0.210 0.188 , 0.219	Depositor DCC
R_{free} test set	4252 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	25.8	Xtriage
Anisotropy	0.259	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 41.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7800	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.15% 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 (i)

5.1 Standard geometry (i)

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	1/1438 (0.1%)	0.88	3/1931 (0.2%)
1	B	0.96	1/1456 (0.1%)	0.93	3/1953 (0.2%)
1	C	0.92	2/1470 (0.1%)	0.91	4/1972 (0.2%)
1	D	0.79	0/1455	0.83	4/1953 (0.2%)
1	E	0.70	0/1419	0.84	3/1907 (0.2%)
All	All	0.85	4/7238 (0.1%)	0.88	17/9716 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	97	GLU	CD-OE2	8.82	1.35	1.25
1	C	109	TYR	CB-CG	5.77	1.60	1.51
1	C	109	TYR	CG-CD2	5.13	1.45	1.39
1	B	75	ASN	C-O	5.01	1.32	1.23

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	190	LEU	CB-CG-CD2	-7.37	98.47	111.00
1	B	77	ASP	N-CA-CB	7.08	123.35	110.60
1	D	77	ASP	CB-CG-OD1	7.08	124.67	118.30
1	E	77	ASP	CB-CG-OD1	6.93	124.54	118.30
1	D	144	LYS	CD-CE-NZ	6.70	127.11	111.70

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	1430	0	1481	3	1
1	B	1448	0	1507	8	1
1	C	1459	0	1523	3	0
1	D	1441	0	1500	6	0
1	E	1411	0	1460	6	2
2	A	152	0	0	1	0
2	B	171	0	0	0	0
2	C	159	0	0	3	0
2	D	98	0	0	0	0
2	E	31	0	0	0	0
All	All	7800	0	7471	25	2

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 2.

The worst 5 of 25 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:B:76:LEU:HD11	1:B:114:GLU:HG3	1.29	1.09
1:D:184:ILE:HD11	1:D:190:LEU:HD11	1.52	0.90
1:E:180:ILE:O	1:E:184:ILE:HD12	1.78	0.83
1:D:184:ILE:HD11	1:D:190:LEU:CD1	2.15	0.76
1:D:184:ILE:CD1	1:D:190:LEU:HD11	2.17	0.74

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	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:ASP:OD2	1:E:174:TYR:OH[1_655]	1.67	0.53
1:B:211:ASP:OD1	1:E:35:GLU:OE2[4_666]	2.19	0.01

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	191/230 (83%)	188 (98%)	3 (2%)	0	100	100
1	B	193/230 (84%)	192 (100%)	1 (0%)	0	100	100
1	C	195/230 (85%)	190 (97%)	5 (3%)	0	100	100
1	D	193/230 (84%)	191 (99%)	2 (1%)	0	100	100
1	E	188/230 (82%)	185 (98%)	3 (2%)	0	100	100
All	All	960/1150 (84%)	946 (98%)	14 (2%)	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	149/179 (83%)	146 (98%)	3 (2%)	55	40
1	B	151/179 (84%)	148 (98%)	3 (2%)	55	40
1	C	153/179 (86%)	151 (99%)	2 (1%)	69	58
1	D	151/179 (84%)	147 (97%)	4 (3%)	46	30
1	E	147/179 (82%)	145 (99%)	2 (1%)	67	55
All	All	751/895 (84%)	737 (98%)	14 (2%)	57	43

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	26	SER
1	C	113	GLU
1	E	214	LYS
1	B	140	GLN
1	E	190	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	140	GLN
1	B	141	ASN
1	E	141	ASN
1	D	141	ASN
1	A	141	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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	193/230 (83%)	-0.42	0	100	100	17, 30, 51, 75	0
1	B	195/230 (84%)	-0.18	0	100	100	15, 26, 50, 64	0
1	C	196/230 (85%)	-0.31	0	100	100	16, 25, 51, 76	0
1	D	193/230 (83%)	0.04	12 (6%)	20	20	19, 36, 70, 98	0
1	E	190/230 (82%)	0.49	19 (10%)	7	6	27, 53, 97, 119	0
All	All	967/1150 (84%)	-0.08	31 (3%)	47	45	15, 32, 75, 119	0

The worst 5 of 31 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	182	PHE	7.1
1	E	150	LEU	6.4
1	D	172	ALA	5.3
1	E	188	ALA	4.6
1	E	174	TYR	4.3

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 monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.