

Full wwPDB X-ray Structure Validation Report (i)

May 17, 2020 - 03:37 am BST

PDB ID	:	4CBP
Title	:	Crystal structure of neural ectodermal development factor IMP-L2.
Authors	:	Kulahin, N.; Kristensen, O.; Brzozowski, M.; Schluckebier, G.; Meyts, P.D.
Deposited on	:	2013-10-15
Resolution	:	1.60 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 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:

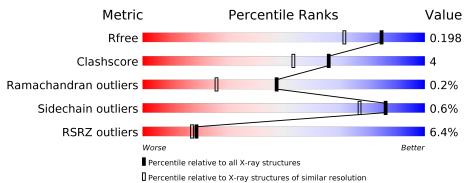
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
$\rm CCP4$:	$7.0.044 (\mathrm{Gargrove})$
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 1.60 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	$egin{array}{llllllllllllllllllllllllllllllllllll$	${f Similar\ resolution}\ (\#{ m Entries},{ m resolution\ range}({ m \AA}))$
R _{free}	130704	3398 (1.60-1.60)
Clashscore	141614	3665(1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563(1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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	А	268	4% 69%	8%	23%
1	В	268	<mark>6%</mark> 71%	6%	23%



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3869 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 NEURAL/ECTODERMAL DEVELOPMENT FACTOR IMP-L2.

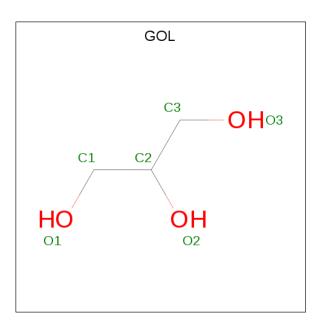
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
1	А	207	Total 1715	C 1069		0 315			0	8	0
1	В	206	Total 1675	C 1051				Se 4	0	5	0

Chain	Residue	Modelled	Actual	Comment	Reference
A	243	GLU	-	expression tag	UNP Q09024
A	244	VAL	-	expression tag	UNP Q09024
A	245	LEU	-	expression tag	UNP Q09024
A	246	PHE	-	expression tag	UNP Q09024
A	247	GLN	-	expression tag	UNP Q09024
В	243	GLU	-	expression tag	UNP Q09024
В	244	VAL	-	expression tag	UNP Q09024
В	245	LEU	-	expression tag	UNP Q09024
В	246	PHE	-	expression tag	UNP Q09024
В	247	GLN	_	expression tag	UNP Q09024

There are 10 discrepancies between the modelled and reference sequences:

• Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0

• Molecule 3 is water.

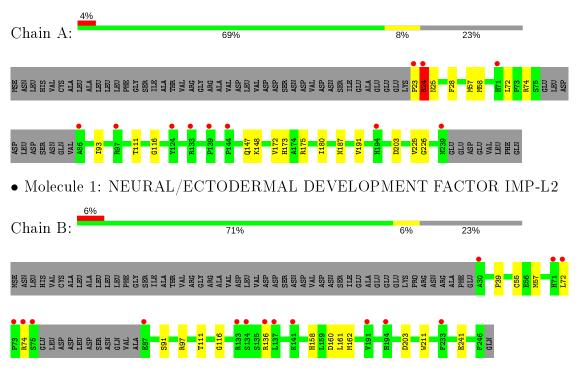
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	249	$\begin{array}{cc} {\rm Total} & {\rm O} \\ 257 & 257 \end{array}$	0	8
3	В	208	Total O 210 210	0	2



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 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: NEURAL/ECTODERMAL DEVELOPMENT FACTOR IMP-L2





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	49.86Å 99.73 Å 56.28 Å	Deperitor
a, b, c, α , β , γ	90.00° 91.99° 90.00°	Depositor
Resolution (Å)	29.54 - 1.60	Depositor
Resolution (A)	37.96 - 1.59	EDS
% Data completeness	$94.7\ (29.54\text{-}1.60)$	Depositor
(in resolution range)	$95.5\ (37.96 ext{-}1.59)$	EDS
R _{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.27 (at 1.59 \text{\AA})$	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.156 , 0.188	Depositor
II, II, <i>free</i>	0.171 , 0.198	DCC
R_{free} test set	1993 reflections (2.83%)	wwPDB-VP
Wilson B-factor $(Å^2)$	18.5	Xtriage
Anisotropy	0.338	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.39 , 59.2	EDS
L-test for twinning ²	$< L > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3869	wwPDB-VP
Average B, all atoms $(Å^2)$	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 10.93% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

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: GOL

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		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.30	0/1748	0.56	0/2367	
1	В	0.31	0/1708	0.51	0/2316	
All	All	0.31	0/3456	0.53	0/4683	

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	А	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Group
1	А	24	ARG	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	А	1715	0	1708	17	0
1	В	1675	0	1664	10	1
2	А	12	0	16	1	0
3	А	257	0	0	6	1
3	В	210	0	0	3	0
All	All	3869	0	3388	27	1

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 4.

All (27) close contacts	within the	he same	$\operatorname{asymmetric}$	unit	are liste	d below,	sorted by	their	clash
magnitude.									

Atom-1	Atom-2	Interatomic $distance (\&)$	Clash
		distance $(Å)$	$\frac{\text{overlap}(\text{\AA})}{0.00}$
1:A:72:LEU:HD21	1:A:111[A]:THR:HG21	1.50	0.90
1:A:203:ASP:OD1	3:A:2180:HOH:O	1.92	0.87
1:B:203:ASP:OD1	3:B:2143:HOH:O	1.92	0.86
1:A:147:GLN:OE1	1:A:175:ARG:NH1	2.14	0.79
1:A:24:ARG:HA	3:A:2001:HOH:O	2.05	0.57
1:A:148:LYS:NZ	3:A:2159:HOH:O	2.24	0.55
1:A:23:PRO:O	1:A:25:ASN:N	2.36	0.53
1:B:72[A]:LEU:HD11	1:B:111[A]:THR:HG21	1.91	0.53
1:B:72[B]:LEU:HG	1:B:111[B]:THR:HG21	1.91	0.52
1:B:91:SER:HB2	1:B:161:LEU:HG	1.94	0.50
1:B:74:ARG:NH1	3:B:2068:HOH:O	2.26	0.49
1:A:187[B]:ASN:ND2	3:A:2207[B]:HOH:O	2.46	0.49
1:A:72:LEU:HD23	1:A:72:LEU:HA	1.71	0.48
1:A:191:VAL:HG22	2:A:1241:GOL:H11	1.95	0.47
1:B:97:ARG:NH2	3:B:2040:HOH:O	2.44	0.47
1:B:158:HIS:CD2	1:B:160:ASP:HB2	2.51	0.46
1:A:57:MSE:SE	1:A:116:GLY:HA3	2.65	0.45
1:B:162:MSE:HE1	1:B:211:TRP:HB2	1.98	0.45
1:A:74:ARG:NH1	3:A:2083:HOH:O	2.47	0.45
1:B:39:PRO:HD3	1:B:55[B]:CYS:SG	2.56	0.45
1:A:147:GLN:NE2	1:A:173:HIS:HE1	2.14	0.44
1:A:148:LYS:HZ2	1:A:226:GLY:HA3	1.82	0.43
1:A:74:ARG:NH1	3:A:2084:HOH:O	2.33	0.42
1:A:23:PRO:HB2	1:A:28:PHE:HB2	2.02	0.42
1:A:172:VAL:HG21	1:A:180:ILE:HD11	2.02	0.41
1:B:57:MSE:SE	1:B:116:GLY:HA3	2.70	0.41
1:A:58:MSE:HE2	1:A:93:ILE:HG22	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-



metry operator and	encoded unit-cell	translations to	be applied.
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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:GLU:OE2	3:A:2034:HOH:O[2_547]	2.16	0.04

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	А	213/268~(80%)	207~(97%)	5(2%)	1 (0%)	29 11
1	В	208/268~(78%)	203~(98%)	5(2%)	0	100 100
All	All	421/536 (78%)	410 (97%)	10 (2%)	1 (0%)	47 26

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	24	ARG

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	Analysed Rotameric Outliers		Percentiles		
1	А	191/230~(83%)	190~(100%)	1 (0%)	88 80		
1	В	188/230~(82%)	187 (100%)	1 (0%)	88 80		
All	All	379/460~(82%)	377(100%)	2(0%)	86 80		

All (2) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	А	225	VAL
1	В	136	ARG

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

Mol	Chain	Res	Type
1	А	173	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)

2 ligands are 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	True	Chain	Dec	Link	B	ond leng	gths	В	ond ang	gles
	Type	Unam	Res	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	А	1241	-	$5,\!5,\!5$	0.28	0	$5,\!5,\!5$	0.26	0
2	GOL	А	1240	-	$5,\!5,\!5$	0.38	0	$5,\!5,\!5$	0.44	0

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	GOL	А	1241	-	-	2/4/4/4	-
2	GOL	А	1240	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	А	1240	GOL	C1-C2-C3-O3
2	А	1240	GOL	O2-C2-C3-O3
2	А	1241	GOL	O1-C1-C2-C3
2	А	1241	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	А	1241	GOL	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		$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q<0.9
1	А	203/268~(75%)	0.25	11 (5%) 25 2	23	11, 22, 41, 56	0
1	В	202/268~(75%)	0.39	15 (7%) 14 1	.3	11, 23, 47, 65	0
All	All	405/536~(75%)	0.32	26 (6%) 19 1	.7	11, 23, 43, 65	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	87	GLU	5.4
1	В	75	SER	5.4
1	В	73	PRO	5.3
1	В	136	ARG	4.6
1	А	144	PRO	3.9
1	А	194	HIS	3.9
1	В	74	ARG	3.6
1	В	133	ARG	3.5
1	В	194	HIS	3.5
1	А	133	ARG	3.3
1	А	24	ARG	3.2
1	В	30	ALA	3.1
1	А	124	TYR	3.1
1	А	86	ALA	3.0
1	В	191	VAL	3.0
1	А	71	HIS	3.0
1	В	134	SER	3.0
1	А	23	PRO	2.9
1	В	137	LEU	2.7
1	В	71[A]	HIS	2.6
1	А	97[A]	ARG	2.6
1	А	239	ASN	2.4
1	В	141	LYS	2.3
1	А	139	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	В	72[A]	LEU	2.2
1	В	233	PHE	2.0

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. 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	\mathbf{RSR}	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	$\mathbf{Q}{<}0.9$
2	GOL	А	1241	6/6	0.84	0.20	$37,\!39,\!39,\!40$	0
2	GOL	А	1240	6/6	0.87	0.17	$39,\!48,\!48,\!49$	0

6.5 Other polymers (i)

There are no such residues in this entry.

