wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 07:10 PM GMT

PDB ID	:	1EBP
Title	:	COMPLEX BETWEEN THE EXTRACELLULAR DOMAIN OF ERYTHROPOIETIN (EPO) RECEPTOR [EBP] AND AN AGONIST PEPTIDE [EMP1]
Authors	:	Livnah, O.; Stura, E.A.; Wilson, I.A.
Deposited on	:	1996-05-07
Resolution	:	2.80 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

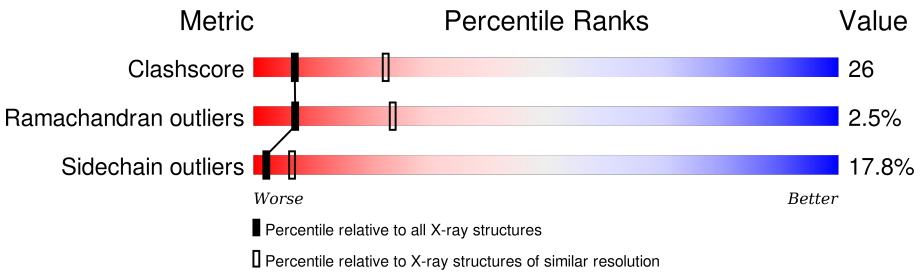
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.80 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))
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	211	57% 33% 9% •
1	B	211	45% 41% 13% •
2	C	20	40% 40% 20%
2	D	20	35% 40% 5% 20%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3546 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 EPO RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	211	1643	1044	291	301	7	0	0	0
1	B	211	1643	1044	291	301	7	0	0	0

- Molecule 2 is a protein called EPO MIMETICS PEPTIDE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	16	130	86	21	21	2	0	0	0
2	D	16	130	86	21	21	2	0	0	0

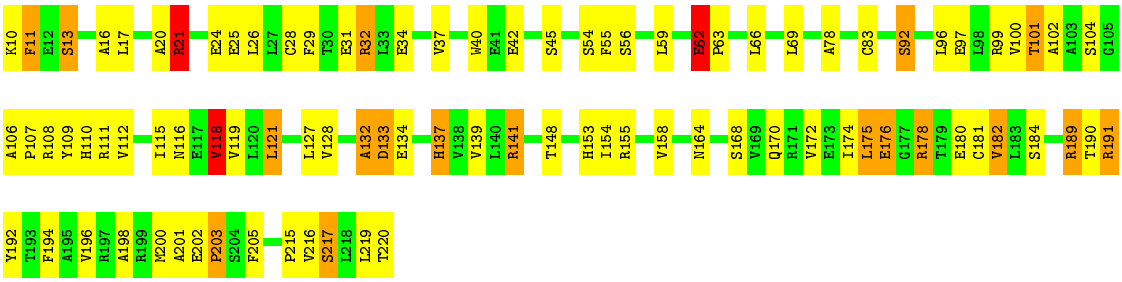
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

Note EDS was not executed.

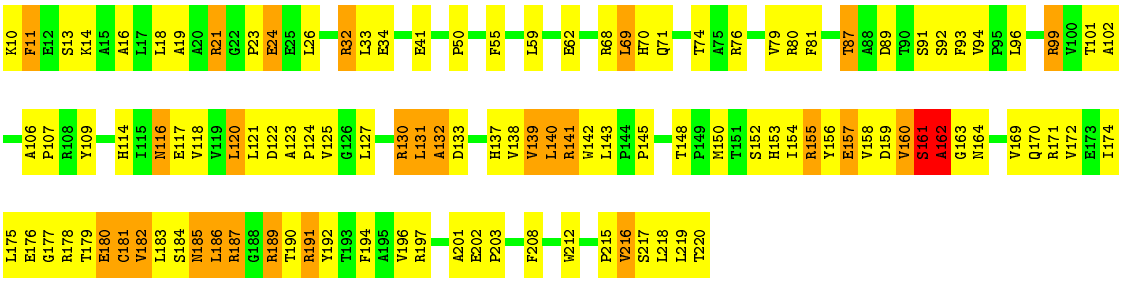
- Molecule 1: EPO RECEPTOR

Chain A: 57% 33% 9%



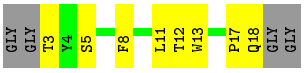
- Molecule 1: EPO RECEPTOR

Chain B: 45% 41% 13%



- Molecule 2: EPO MIMETICS PEPTIDE 1

Chain C: 40% 40% 20%



- Molecule 2: EPO MIMETICS PEPTIDE 1

Chain D: 35% 40% 5% 20%

GLY
GLY
T3
Y4
S5
C6
H7
F8
W13
V14
C15
K16
P17
Q18
GLY
GLY

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	59.24Å 75.50Å 132.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.210 , 0.334	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3546	wwPDB-VP
Average B, all atoms ($Å^2$)	13.0	wwPDB-VP

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	0.82	0/1687	0.99	5/2300 (0.2%)
1	B	0.92	1/1687 (0.1%)	1.07	9/2300 (0.4%)
2	C	0.76	0/136	0.93	0/186
2	D	0.70	0/136	1.03	0/186
All	All	0.86	1/3646 (0.0%)	1.03	14/4972 (0.3%)

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	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	162	ALA	N-CA	19.76	1.85	1.46

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	162	ALA	N-CA-C	-9.41	85.59	111.00
1	B	191	ARG	NE-CZ-NH2	7.58	124.09	120.30
1	A	21	ARG	NE-CZ-NH2	7.43	124.01	120.30
1	B	161	SER	C-N-CA	-7.00	104.19	121.70
1	B	189	ARG	NE-CZ-NH2	6.88	123.74	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	161	SER	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	A	1643	0	1606	59	0
1	B	1643	0	1606	117	0
2	C	130	0	119	6	0
2	D	130	0	119	8	0
All	All	3546	0	3450	185	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 26.

The worst 5 of 185 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:162:ALA:CA	1:B:162:ALA:N	1.85	1.39
1:B:10:LYS:HA	1:B:13:SER:HB3	1.32	1.12
1:B:155:ARG:NH2	1:B:175:LEU:HG	1.76	1.01
1:A:99:ARG:HG2	1:A:110:HIS:HD2	1.27	0.98
1:B:141:ARG:HE	1:B:180:GLU:HB2	1.28	0.96

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	209/211 (99%)	187 (90%)	17 (8%)	5 (2%)	7 25
1	B	209/211 (99%)	176 (84%)	28 (13%)	5 (2%)	7 25
2	C	14/20 (70%)	14 (100%)	0	0	100 100
2	D	14/20 (70%)	12 (86%)	1 (7%)	1 (7%)	1 3
All	All	446/462 (96%)	389 (87%)	46 (10%)	11 (2%)	7 24

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	162	ALA
1	B	164	ASN
1	A	132	ALA
1	A	164	ASN
2	D	13	TRP

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	173/173 (100%)	137 (79%)	36 (21%)	1 4
1	B	173/173 (100%)	144 (83%)	29 (17%)	2 8
2	C	15/15 (100%)	13 (87%)	2 (13%)	5 14
2	D	15/15 (100%)	15 (100%)	0	100 100
All	All	376/376 (100%)	309 (82%)	67 (18%)	2 6

5 of 67 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	196	VAL
1	B	18	LEU
1	B	185	ASN
1	A	203	PRO
1	A	217	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	52	ASN
1	B	116	ASN
1	B	153	HIS
1	A	170	GLN
1	B	137	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)

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)

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates (i)

EDS was not executed - this section will therefore be empty.

6.4 Ligands (i)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers (i)

EDS was not executed - this section will therefore be empty.