



wwPDB X-ray Structure Validation Summary Report ⓘ

May 21, 2020 – 01:03 pm BST

PDB ID : 6JOD
Title : Angiotensin II type 2 receptor with ligand
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Deposited on : 2019-03-20
Resolution : 3.20 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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

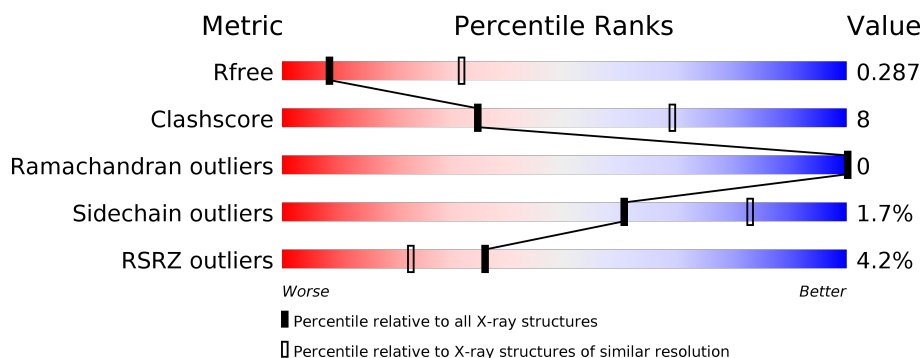
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 $\leq 5\%$. 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	312	<div> <div>5%</div> <div> <div></div> <div>74%</div> <div>23%</div> <div>••</div> </div> </div>
2	B	8	<div> <div>38%</div> <div>50%</div> <div>13%</div> </div>
3	C	86	<div> <div>16%</div> <div>62%</div> <div>6%</div> <div>•</div> <div>31%</div> </div>
4	H	220	<div> <div>%</div> <div>82%</div> <div>18%</div> </div>
5	L	212	<div> <div>80%</div> <div>20%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6257 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 Type-2 angiotensin II receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	306	Total	C	N	O	S	0	0	0
			2470	1662	390	397	21			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	208	ALA	SER	engineered mutation	UNP P50052

- Molecule 2 is a protein called Angiotensin II.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	8	Total	C	N	O	0	0	0
			75	50	13	12			

- Molecule 3 is a protein called Soluble cytochrome b562,Soluble cytochrome b562.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	59	Total	C	N	O	S	0	0	0
			438	269	77	91	1			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1007	TRP	MET	engineered mutation	UNP P0ABE7
C	1061	GLY	-	linker	UNP P0ABE7
C	1062	SER	-	linker	UNP P0ABE7
C	1063	GLY	-	linker	UNP P0ABE7
C	1064	SER	-	linker	UNP P0ABE7
C	1065	GLY	-	linker	UNP P0ABE7
C	1066	ASP	-	linker	UNP P0ABE7
C	1098	ILE	ARG	engineered mutation	UNP P0ABE7
C	1102	ILE	HIS	engineered mutation	UNP P0ABE7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1106	GLY	ARG	engineered mutation	UNP P0ABE7

- Molecule 4 is a protein called Heavy chain of 4A03Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	220	Total	C	N	O	S	0	0	0
			1643	1046	265	323	9			

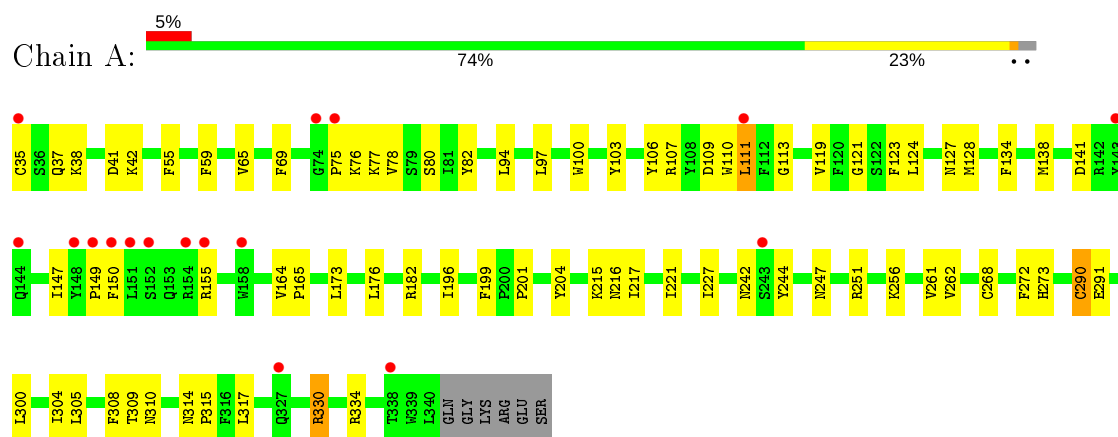
- Molecule 5 is a protein called Light chain of 4A03Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	L	212	Total	C	N	O	S	0	0	0
			1631	1017	269	336	9			

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.

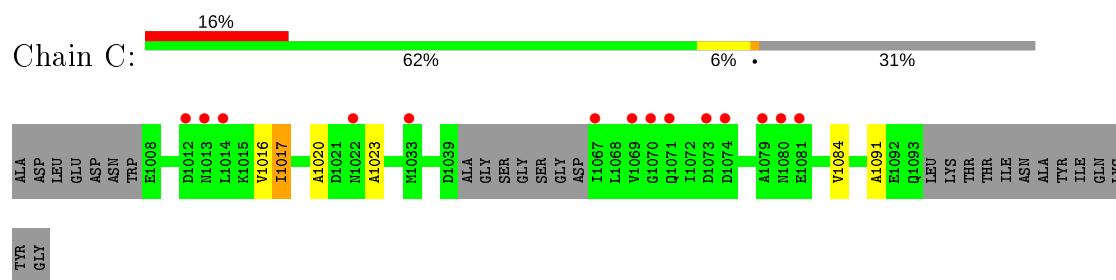
- Molecule 1: Type-2 angiotensin II receptor



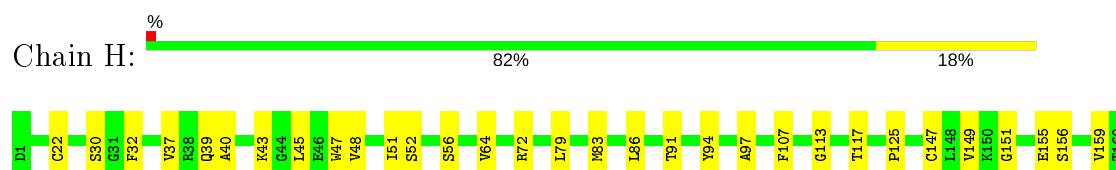
- Molecule 2: Angiotensin II

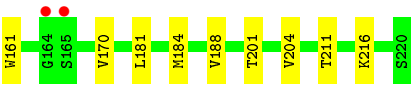


- Molecule 3: Soluble cytochrome b562, Soluble cytochrome b562

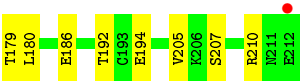
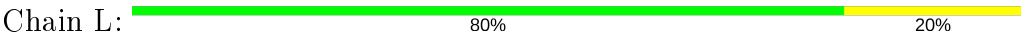


- Molecule 4: Heavy chain of 4A03Fab





● Molecule 5: Light chain of 4A03Fab



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	102.55Å 426.43Å 52.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.85 – 3.20 49.85 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.85-3.20) 99.9 (49.85-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.11.1 _2575	Depositor
R, R_{free}	0.235 , 0.287 0.235 , 0.287	Depositor DCC
R_{free} test set	940 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å ²)	122.1	Xtriage
Anisotropy	0.403	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 87.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6257	wwPDB-VP
Average B, all atoms (Å ²)	141.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

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	0.27	0/2546	0.42	0/3472
2	B	0.24	0/78	0.44	0/104
3	C	0.23	0/436	0.35	0/584
4	H	0.29	0/1690	0.50	0/2311
5	L	0.29	0/1669	0.48	0/2269
All	All	0.28	0/6419	0.46	0/8740

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	2470	0	2538	52	0
2	B	75	0	71	5	0
3	C	438	0	452	3	0
4	H	1643	0	1592	25	0
5	L	1631	0	1561	24	0
All	All	6257	0	6214	104	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 8.

The worst 5 of 104 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:261:VAL:HA	1:A:317:LEU:HD21	1.63	0.79
4:H:170:VAL:HG22	4:H:188:VAL:HG22	1.67	0.77
5:L:186:GLU:HA	5:L:210:ARG:HH12	1.49	0.76
1:A:69:PHE:HE2	1:A:80:SER:HB3	1.55	0.70
4:H:201:THR:HG22	4:H:216:LYS:HA	1.79	0.64

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	304/312 (97%)	293 (96%)	11 (4%)	0	100	100
2	B	6/8 (75%)	6 (100%)	0	0	100	100
3	C	55/86 (64%)	55 (100%)	0	0	100	100
4	H	218/220 (99%)	209 (96%)	9 (4%)	0	100	100
5	L	210/212 (99%)	203 (97%)	7 (3%)	0	100	100
All	All	793/838 (95%)	766 (97%)	27 (3%)	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	270/275 (98%)	261 (97%)	9 (3%)	38	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	8/8 (100%)	7 (88%)	1 (12%)	4	21
3	C	44/64 (69%)	43 (98%)	1 (2%)	50	78
4	H	185/185 (100%)	185 (100%)	0	100	100
5	L	187/187 (100%)	186 (100%)	1 (0%)	88	95
All	All	694/719 (96%)	682 (98%)	12 (2%)	60	83

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	244	TYR
1	A	290	CYS
2	B	5	ILE
1	A	150	PHE
1	A	330	ARG

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

Mol	Chain	Res	Type
1	A	216	ASN
1	A	273	HIS
5	L	123	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	306/312 (98%)	0.13	17 (5%) 24 13	87, 143, 256, 323	0
2	B	8/8 (100%)	-0.11	0 100 100	117, 134, 153, 176	0
3	C	59/86 (68%)	1.36	14 (23%) 0 0	187, 251, 300, 348	0
4	H	220/220 (100%)	0.05	2 (0%) 84 75	76, 109, 168, 276	0
5	L	212/212 (100%)	-0.01	1 (0%) 91 86	73, 111, 151, 182	0
All	All	805/838 (96%)	0.16	34 (4%) 36 23	73, 126, 259, 348	0

The worst 5 of 34 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	1080	ASN	6.0
4	H	165	SER	5.8
1	A	152	SER	4.9
1	A	150	PHE	4.7
4	H	164	GLY	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 carbohydrates 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.