wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 05:14 AM GMT

PDB ID	:	2PZX
Title	:	Structure of the methuselah ectodomain with peptide inhibitor
Authors	:	West Jr., A.P.; Ja, W.W.; Delker, S.L.; Bjorkman, P.J.; Benzer, S.; Roberts, R.W.
Deposited on	:	2007-05-18
Resolution	:	3.50 Å(reported)

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

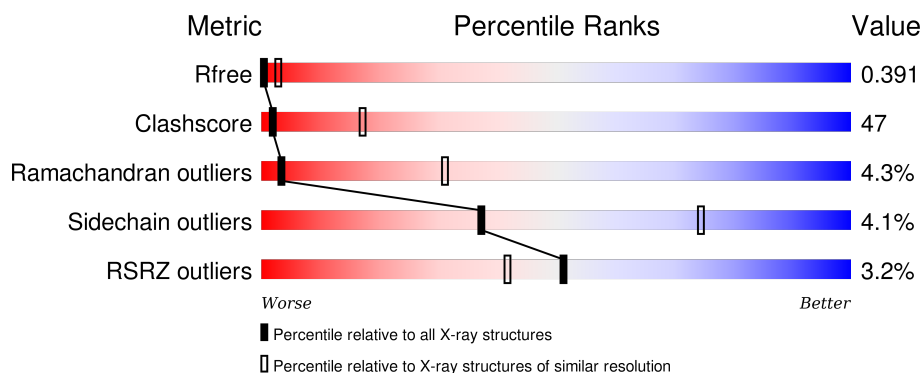|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 3.50 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}	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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.

Mol	Chain	Length	Quality of chain
1	A	188	5% / 40% 54% 6%
1	B	188	5% / 41% 52% 6%
1	C	188	% / 38% 55% 6%
1	D	188	2% / 41% 53% 6%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 9174 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 G-protein coupled receptor Mth.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	188	Total	C	N	O	S	0	0	0
			1529	965	262	288	14			
1	B	188	Total	C	N	O	S	0	0	0
			1529	965	262	288	14			
1	C	188	Total	C	N	O	S	0	188	0
			3058	1930	524	576	28			
1	D	188	Total	C	N	O	S	0	188	0
			3058	1930	524	576	28			

3 Residue-property plots ⓘ

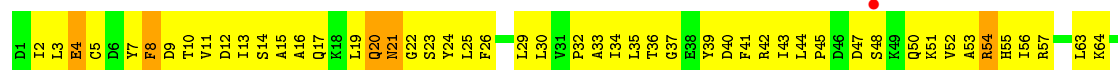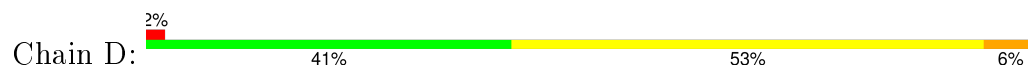These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

• Molecule 1: G-protein coupled receptor Mth

• Molecule 1: G-protein coupled receptor Mth

• Molecule 1: G-protein coupled receptor Mth

R151 D154 R155 V156 T157 L158 R159 K160 R161 E162 Y163 C164 L165 Q166 H167 L168 T169 D172 G173 N174 A175 T176 S177 I178 R179 I180 A181 P182 H183 N184 C185 L186 I187 V188

• Molecule 1: G-protein coupled receptor Mth

Chain D:

2%

41%　　　　　　　　　　　　　　　53%　　　　　　　6%

D1 I2 L3 E4 C5 D6 Y7 F8 D9 T10 V11 D12 I13 S14 A15 A16 Q17 K18 L19 Q20 N21 G22 S23 Y24 L25 F26 L29 L30 V31 P32 A33 I34 L35 T36 G37 E38 Y39 D40 F41 R42 I43 L44 P45 D46 D47 S48 K49 Q50 K51 V52 A53 R54 H55 I56 R57 L63 K64

V67 R68 F69 C70 C71 P72 I76 M77 V81 C82 Y83 M86 L91 L94 D95 P96 F97 L98 N99 V100 D103 R109 R110 H111 F112 K113 N114 E115 L116 Q119 P123 M124 P125 C126 M129 F130 Y131 L132 D133 N134 R135 D139 L143 F149 F150 R151

D154 R155 V156 T157 L158 R159 K160 R161 E162 Y163 C164 L165 Q166 T169 D172 G173 N174 A175 T176 S177 I178 R179 I180 A181 P182 H183 N184 C185 L186 I187 V188

4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 42	Depositor
Cell constants a, b, c, α, β, γ	94.23Å 94.23Å 173.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.99 – 3.50 29.80 – 3.30	Depositor EDS
% Data completeness (in resolution range)	96.5 (7.99-3.50) 95.9 (29.80-3.30)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.59 (at 3.31Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.376 , 0.407 0.351 , 0.391	Depositor DCC
R_{free} test set	822 reflections (5.12%)	DCC
Wilson B-factor (Å^2)	58.6	Xtriage
Anisotropy	0.831	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.17 , 5.5	EDS
Estimated twinning fraction	0.368 for h,-k,-l	Xtriage
L-test for twinning[2]	$< |L| > = 0.43, < L^2 > = 0.25$	Xtriage
Outliers	5 of 21889 reflections (0.023%)	Xtriage
F_o,F_c correlation	0.81	EDS
Total number of atoms	9174	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 70.08 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.3188e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

---

[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.35	0/1564	0.64	0/2115
1	B	0.35	0/1564	0.64	0/2115
1	C	0.35	0/3128	0.64	0/4230
1	D	0.35	0/3128	0.64	0/4230
All	All	0.35	0/9384	0.64	0/12690

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	1529	0	1459	145	3
1	B	1529	0	1459	142	3
1	C	3058	0	2883	301	2
1	D	3058	0	2883	285	2
All	All	9174	0	8684	836	6

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 47.

The worst 5 of 836 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:D:77[A]:MET:HA	1:D:77[A]:MET:HE3	1.44	0.98
1:C:4[B]:GLU:HB2	1:D:3[B]:LEU:HD13	1.49	0.94
1:C:3[B]:LEU:HD12	1:D:3[B]:LEU:HG	1.54	0.89
1:C:115[B]:GLU:O	1:C:116[B]:LEU:HD23	1.77	0.85
1:C:115[A]:GLU:O	1:C:116[A]:LEU:HD23	1.77	0.85

The worst 5 of 6 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:187:ILE:O	1:A:187:ILE:O[2_665]	1.92	0.28
1:B:109:ARG:NH2	1:D:109[B]:ARG:NH2[3_654]	1.95	0.25
1:B:187:ILE:O	1:B:187:ILE:O[2_665]	1.97	0.23
1:A:109:ARG:NH2	1:C:109[A]:ARG:NH2[3_655]	1.98	0.22
1:B:91:LEU:O	1:D:91[B]:LEU:O[3_654]	2.08	0.12

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	186/188 (99%)	153 (82%)	25 (13%)	8 (4%)	3	31
1	B	186/188 (99%)	153 (82%)	25 (13%)	8 (4%)	3	31
1	C	372/188 (198%)	306 (82%)	50 (13%)	16 (4%)	3	31
1	D	372/188 (198%)	306 (82%)	50 (13%)	16 (4%)	3	31
All	All	1116/752 (148%)	918 (82%)	150 (13%)	48 (4%)	3	31

5 of 48 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	A	8	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	160	LYS
1	B	4	GLU
1	B	8	PHE

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	171/171 (100%)	164 (96%)	7 (4%)	37	74
1	B	171/171 (100%)	164 (96%)	7 (4%)	37	74
1	C	342/171 (200%)	328 (96%)	14 (4%)	37	74
1	D	342/171 (200%)	328 (96%)	14 (4%)	37	74
All	All	1026/684 (150%)	984 (96%)	42 (4%)	37	74

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	68[A]	ARG
1	C	77[B]	MET
1	D	94[A]	LEU
1	C	68[B]	ARG
1	C	69[B]	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	184	ASN
1	B	20	GLN
1	B	166	GLN
1	A	183	HIS
1	B	138	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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, 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	188/188 (100%)	0.30	9 (4%)	34	27	0, 44, 148, 196	0
1	B	188/188 (100%)	0.30	9 (4%)	34	27	0, 44, 148, 196	0
1	C	188/188 (100%)	0.07	2 (1%)	82	73	0, 44, 148, 196	0
1	D	188/188 (100%)	0.08	4 (2%)	67	58	0, 44, 148, 196	0
All	All	752/752 (100%)	0.19	24 (3%)	51	42	0, 44, 150, 196	0

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	174	ASN	8.9
1	A	174	ASN	7.7
1	C	174[A]	ASN	4.0
1	A	137	GLU	3.9
1	A	83	TYR	3.5

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 carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

WORLDWIDE
wwPDB
PROTEIN DATA BANK

6.5 Other polymers (i)

There are no such residues in this entry.