Full wwPDB X-ray Structure Validation Report (i)

Feb 28, 2014 – 04:33 PM GMT

PDB ID   :   3W0G
Title   :   Crystal Structure of Rat VDR Ligand Binding Domain in Complex with Novel Nonsecosteroidal Ligands
Authors   :   Shimizu, T.; Asano, L.; Kuwabara, N.; Ito, I.; Waku, T.; Yanagisawa, J.; Miyachi, H.
Deposited on :   2012-10-30
Resolution :   1.94 Å(reported)

1   Overall quality at a glance ⓘ

The reported resolution of this entry is 1.94 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	Percentile Ranks	Value
Rfree		0.257
Clashscore		6
Ramachandran outliers		0
Sidechain outliers		4.3%
RSRZ outliers		5.5%

Worse   Better

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
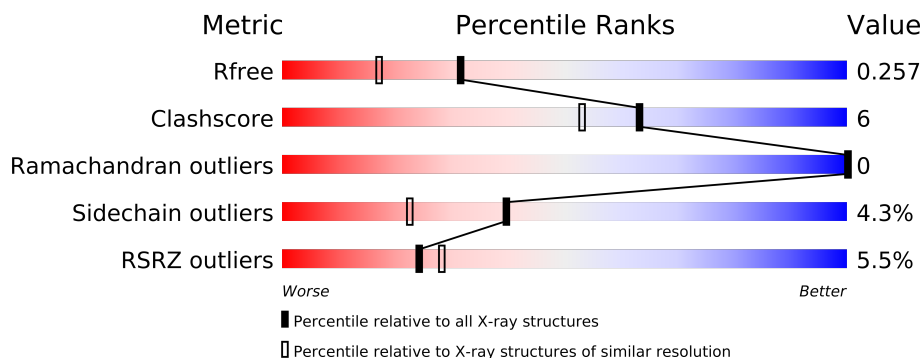
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	2024 (1.96-1.92)
Clashscore	79885	2281 (1.96-1.92)
Ramachandran outliers	78287	2255 (1.96-1.92)
Sidechain outliers	78261	2255 (1.96-1.92)
RSRZ outliers	66119	2024 (1.96-1.92)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	253	
2	C	13	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 2198 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Vitamin D3 receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	242	Total 1949	C 1239	N 335	O 363	S 12	0	1	0

There are 47 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	SER	DELETION	UNP P13053
A	?	-	TYR	DELETION	UNP P13053
A	?	-	SER	DELETION	UNP P13053
A	?	-	PRO	DELETION	UNP P13053
A	?	-	ARG	DELETION	UNP P13053
A	?	-	PRO	DELETION	UNP P13053
A	?	-	THR	DELETION	UNP P13053
A	?	-	LEU	DELETION	UNP P13053
A	?	-	SER	DELETION	UNP P13053
A	?	-	PHE	DELETION	UNP P13053
A	?	-	SER	DELETION	UNP P13053
A	?	-	GLY	DELETION	UNP P13053
A	?	-	ASN	DELETION	UNP P13053
A	?	-	SER	DELETION	UNP P13053
A	?	-	SER	DELETION	UNP P13053
A	?	-	SER	DELETION	UNP P13053
A	?	-	SER	DELETION	UNP P13053
A	?	-	SER	DELETION	UNP P13053
A	?	-	SER	DELETION	UNP P13053
A	?	-	ASP	DELETION	UNP P13053
A	?	-	LEU	DELETION	UNP P13053
A	?	-	TYR	DELETION	UNP P13053
A	?	-	THR	DELETION	UNP P13053
A	?	-	THR	DELETION	UNP P13053
A	?	-	SER	DELETION	UNP P13053
A	?	-	LEU	DELETION	UNP P13053
A	?	-	ASP	DELETION	UNP P13053

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	MET	DELETION	UNP P13053
A	?	-	MET	DELETION	UNP P13053
A	?	-	GLU	DELETION	UNP P13053
A	?	-	PRO	DELETION	UNP P13053
A	?	-	SER	DELETION	UNP P13053
A	?	-	GLY	DELETION	UNP P13053
A	?	-	PHE	DELETION	UNP P13053
A	?	-	SER	DELETION	UNP P13053
A	?	-	ASN	DELETION	UNP P13053
A	?	-	LEU	DELETION	UNP P13053
A	?	-	ASP	DELETION	UNP P13053
A	?	-	LEU	DELETION	UNP P13053
A	?	-	ASN	DELETION	UNP P13053
A	?	-	GLY	DELETION	UNP P13053
A	?	-	GLU	DELETION	UNP P13053
A	?	-	ASP	DELETION	UNP P13053
A	?	-	SER	DELETION	UNP P13053
A	?	-	ASP	DELETION	UNP P13053
A	?	-	ASP	DELETION	UNP P13053
A	?	-	PRO	DELETION	UNP P13053

- Molecule 2 is a protein called Mediator of RNA polymerase II transcription subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	12	99	63	18	16	2	0	0	0

- Molecule 3 is (2S)-3-{4-[2-(4-{[(2R)-2-HYDROXY-3,3-DIMETHYLBUTYL]OXY}PHENYL)PROPAN-2-YL]PHENOXY}PROPANE-1,2-DIOL (three-letter code: W07) (formula: $C_{24}H_{34}O_5$).
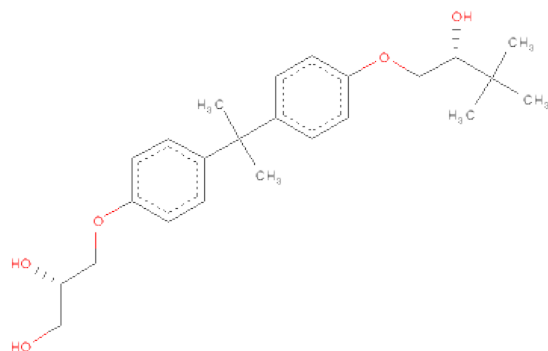
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 29	C 24	O 5	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	116	Total 116	O 116	0	0
4	C	5	Total 5	O 5	0	0

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.
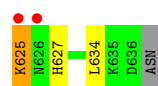
• Molecule 1: Vitamin D3 receptor

Chain A:
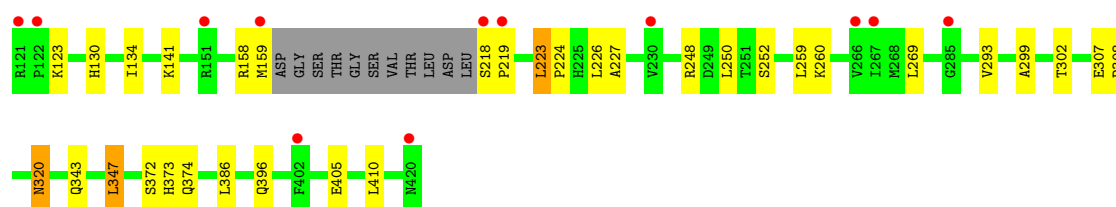
• Molecule 2: Mediator of RNA polymerase II transcription subunit 1

Chain C:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	154.30Å 41.98Å 42.05Å 90.00° 94.86° 90.00°	Depositor
Resolution (Å)	29.60 – 1.94 27.20 – 1.80	Depositor EDS
% Data completeness (in resolution range)	96.9 (29.60-1.94) 97.0 (27.20-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.28 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.214 , 0.258 0.214 , 0.257	Depositor DCC
R_{free} test set	1252 reflections (5.37%)	DCC
Wilson B-factor (Å^2)	34.8	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 42.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Outliers	1 of 24574 reflections (0.004%)	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	2198	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.76% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: W07

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	0.54	0/1989	0.59	0/2690
2	C	0.51	0/100	0.71	0/132
All	All	0.54	0/2089	0.59	0/2822

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts ⓘ

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1949	0	1956	19	0
2	C	99	0	106	6	0
3	A	29	0	34	2	0
4	A	116	0	0	5	0
4	C	5	0	0	0	0
All	All	2198	0	2096	23	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

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All (23) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:141[B]:LYS:HD3	4:A:697:HOH:O	1.95	0.66
1:A:302:THR:H	1:A:396:GLN:HE22	1.45	0.65
1:A:218:SER:HB2	1:A:219:PRO:HD3	1.79	0.62
1:A:405:GLU:HB3	4:A:687:HOH:O	1.99	0.61
1:A:250:LEU:HD23	1:A:347:LEU:HD13	1.84	0.60
2:C:625:LYS:HB2	2:C:627:HIS:HE1	1.66	0.60
1:A:259:LEU:CD1	2:C:634:LEU:HD21	2.35	0.57
2:C:625:LYS:HB2	2:C:627:HIS:CE1	2.43	0.51
1:A:226:LEU:HD12	1:A:299:ALA:HB2	1.91	0.50
1:A:260:LYS:HE3	2:C:627:HIS:NE2	2.28	0.48
1:A:372:SER:O	4:A:659:HOH:O	2.20	0.47
1:A:227:ALA:HA	3:A:501:W07:H29	1.97	0.47
3:A:501:W07:H30	3:A:501:W07:H16	1.70	0.47
1:A:269:LEU:HG	1:A:386:LEU:HD11	1.97	0.46
1:A:373:HIS:CE1	1:A:374:GLN:HG2	2.50	0.46
2:C:625:LYS:HD3	2:C:625:LYS:N	2.30	0.45
1:A:130:HIS:NE2	1:A:134:ILE:HD11	2.30	0.45
1:A:248:ARG:HB3	4:A:667:HOH:O	2.17	0.44
1:A:293:VAL:HG13	4:A:706:HOH:O	2.16	0.44
1:A:223:LEU:HB3	1:A:224:PRO:HD3	2.01	0.42
1:A:307:GLU:HB3	1:A:308:PRO:HD3	2.03	0.41
1:A:320:ASN:HA	1:A:320:ASN:HD22	1.79	0.41
1:A:260:LYS:CE	2:C:627:HIS:NE2	2.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	239/253 (94%)	231 (97%)	8 (3%)	0	100	100
2	C	10/13 (77%)	10 (100%)	0	0	100	100
All	All	249/266 (94%)	241 (97%)	8 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	221/231 (96%)	212 (96%)	9 (4%)	41	24
2	C	12/13 (92%)	11 (92%)	1 (8%)	16	4
All	All	233/244 (96%)	223 (96%)	10 (4%)	40	22

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	123	LYS
1	A	158	ARG
1	A	159	MET
1	A	223	LEU
1	A	252	SER
1	A	320	ASN
1	A	343	GLN
1	A	347	LEU
1	A	410	LEU
2	C	625	LYS

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	255	GLN
1	A	320	ASN
1	A	396	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

1 ligand is 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
3	W07	A	501	-	30,30,30	0.71	0	43,43,43	1.28	4 (9%)

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
3	W07	A	501	-	-	0/30/30/30	0/2/2/2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	501	W07	C3-O03-C4	4.92	128.34	117.91
3	A	501	W07	C19-O04-C16	2.64	123.51	117.91
3	A	501	W07	O03-C3-C2	2.47	112.36	107.66
3	A	501	W07	O05-C20-C19	2.37	113.46	107.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers (i)

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 (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(Å²)	Q<0.9
1	A	242/253 (95%)	0.35	12 (4%)	28	32	23, 39, 62, 99	0
2	C	12/13 (92%)	0.75	2 (16%)	2	2	34, 42, 72, 83	0
All	All	254/266 (95%)	0.37	14 (5%)	24	28	23, 40, 63, 99	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	122	PRO	7.6
1	A	218	SER	6.6
1	A	159	MET	5.3
2	C	625	LYS	5.0
1	A	121	ARG	4.8
1	A	402	PHE	4.6
1	A	219	PRO	3.8
1	A	420	ASN	3.7
1	A	285	GLY	3.0
1	A	151	ARG	3.0
1	A	267	ILE	3.0
2	C	626	ASN	2.9
1	A	230	VAL	2.5
1	A	266	VAL	2.2

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	W07	A	501	29/29	0.16	0.72	35,38,41,42	0

6.5 Other polymers (i)

There are no such residues in this entry.