wwPDB X-ray Structure Validation Summary Report (i)

Nov 3, 2016 – 01:37 PM EDT

PDB ID	:	1G5Y
Title	:	THE 2.0 ANGSTROM RESOLUTION CRYSTAL STRUCTURE OF THE RXRALPHA LIGAND BINDING DOMAIN TETRAMER IN THE PRESENCE OF A NON-ACTIVATING RETINOIC ACID ISOMER.
Authors	:	Gampe Jr., R.T.; Montana, V.G.; Lambert, M.H.; Wisely, G.B.; Milburn, M.V.; Xu, H.E.
Deposited on	:	2000-11-02
Resolution	:	2.00 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:

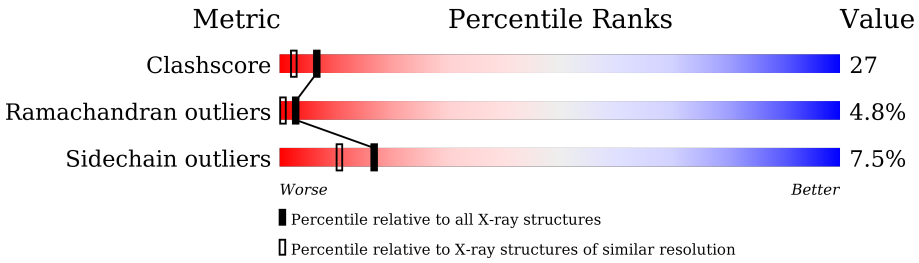
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028320

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 2.00 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	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)

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	238	61% 26% 8%
1	B	238	63% 26% 7%
1	C	238	53% 37% 5%
1	D	238	57% 30% 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	9CR	B	501	-	-	X	-

2 Entry composition

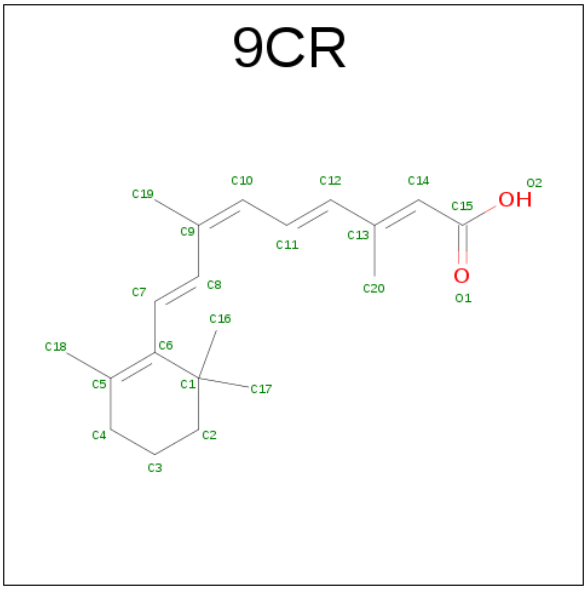
There are 3 unique types of molecules in this entry. The entry contains 7438 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 RETINOIC ACID RECEPTOR RXR-ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	228	Total	C	N	O	S	0	0	0
			1724	1104	301	310	9			
1	B	229	Total	C	N	O	S	0	0	0
			1739	1115	303	312	9			
1	C	226	Total	C	N	O	S	0	0	0
			1704	1093	293	309	9			
1	D	229	Total	C	N	O	S	0	0	0
			1731	1110	301	311	9			

- Molecule 2 is (9CIS)-RETINOIC ACID (three-letter code: 9CR) (formula: $C_{20}H_{28}O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	O		0	0
			22	20	2			
2	C	1	Total	C	O		0	0
			22	20	2			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	138	Total O 138 138	0	0
3	B	145	Total O 145 145	0	0
3	C	99	Total O 99 99	0	0
3	D	114	Total O 114 114	0	0

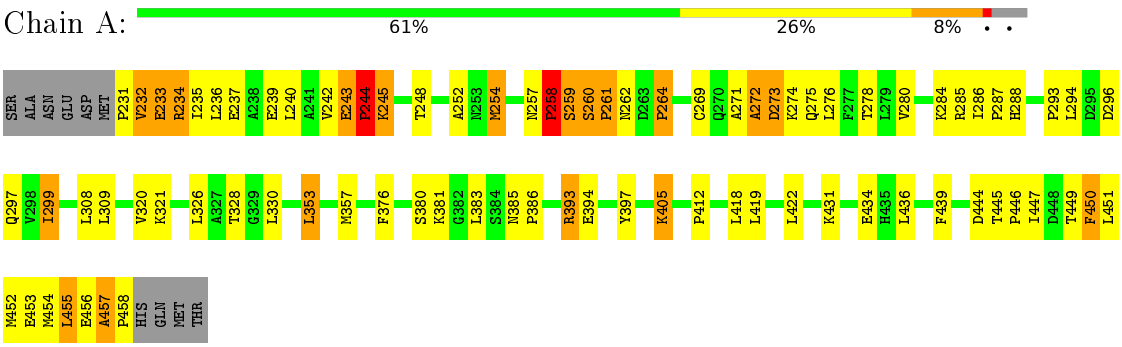
3 Residue-property plots (i)

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.

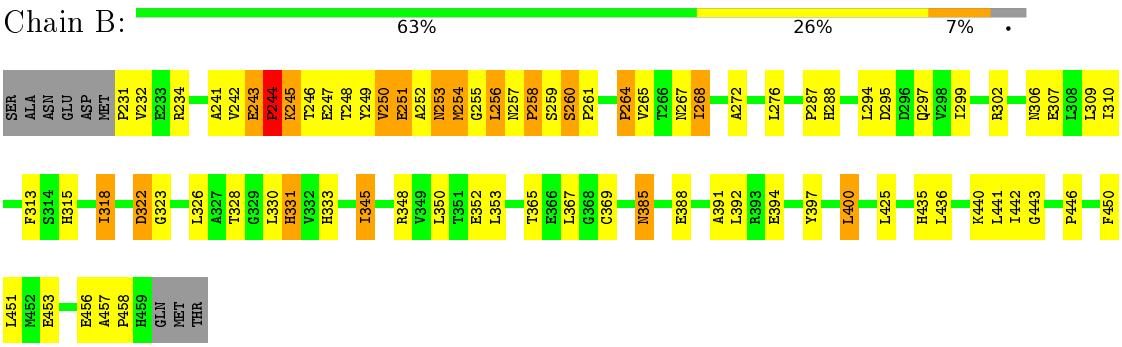
• Molecule 1: RETINOIC ACID RECEPTOR RXR-ALPHA

Chain A:



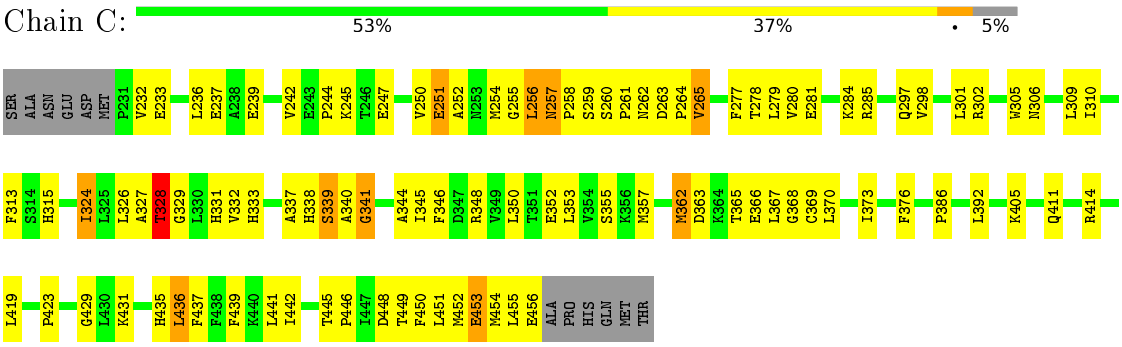
• Molecule 1: RETINOIC ACID RECEPTOR RXR-ALPHA

Chain B:



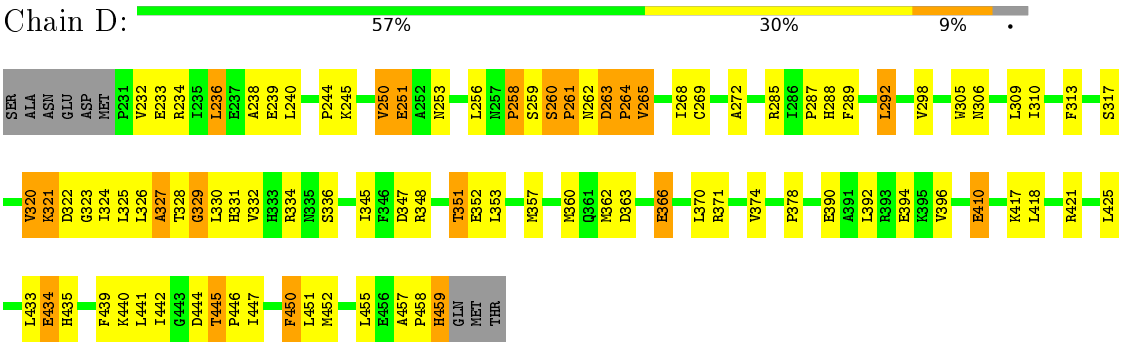
• Molecule 1: RETINOIC ACID RECEPTOR RXR-ALPHA

Chain C:



• Molecule 1: RETINOIC ACID RECEPTOR RXR-ALPHA

Chain D:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	51.05Å 99.70Å 96.28Å 90.00° 96.70° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00	Depositor
% Data completeness (in resolution range)	99.5 (20.00-2.00)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNX 2000	Depositor
R, R_{free}	0.231 , 0.254	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7438	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 9CR

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	0.44	1/1756 (0.1%)	0.72	6/2378 (0.3%)
1	B	0.40	0/1773	0.65	3/2403 (0.1%)
1	C	0.36	0/1736	0.62	3/2356 (0.1%)
1	D	0.40	0/1765	0.70	5/2394 (0.2%)
All	All	0.40	1/7030 (0.0%)	0.67	17/9531 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	233	GLU	CG-CD	5.56	1.60	1.51

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	459	HIS	N-CA-C	-10.31	83.15	111.00
1	A	234	ARG	N-CA-C	-7.46	90.87	111.00
1	B	244	PRO	N-CA-CB	6.41	110.99	103.30
1	D	265	VAL	N-CA-C	-5.79	95.38	111.00
1	D	258	PRO	N-CA-CB	5.78	110.23	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	1724	0	1692	105	0
1	B	1739	0	1719	78	0
1	C	1704	0	1672	106	0
1	D	1731	0	1702	99	0
2	B	22	0	27	14	0
2	C	22	0	27	5	0
3	A	138	0	0	8	0
3	B	145	0	0	2	1
3	C	99	0	0	8	0
3	D	114	0	0	7	1
All	All	7438	0	6839	373	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 27.

The worst 5 of 373 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:232:VAL:HG23	1:A:235:ILE:HD12	1.25	1.09
1:A:233:GLU:HA	1:A:236:LEU:HB3	1.38	1.05
1:A:232:VAL:HG13	3:A:501:HOH:O	1.56	1.04
1:D:327:ALA:N	1:D:331:HIS:NE2	2.10	0.98
1:D:253:ASN:HA	1:D:329:GLY:H	1.26	0.98

All (1) 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)
3:B:554:HOH:O	3:D:492:HOH:O[1_455]	1.79	0.41

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	226/238 (95%)	201 (89%)	14 (6%)	11 (5%)	3 0
1	B	227/238 (95%)	202 (89%)	11 (5%)	14 (6%)	2 0
1	C	224/238 (94%)	196 (88%)	20 (9%)	8 (4%)	4 1
1	D	227/238 (95%)	206 (91%)	11 (5%)	10 (4%)	3 1
All	All	904/952 (95%)	805 (89%)	56 (6%)	43 (5%)	3 0

5 of 43 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	244	PRO
1	A	245	LYS
1	A	258	PRO
1	A	264	PRO
1	A	457	ALA

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	172/205 (84%)	156 (91%)	16 (9%)	11 6
1	B	176/205 (86%)	165 (94%)	11 (6%)	22 16
1	C	172/205 (84%)	161 (94%)	11 (6%)	22 15
1	D	174/205 (85%)	160 (92%)	14 (8%)	15 9
All	All	694/820 (85%)	642 (92%)	52 (8%)	17 11

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	392	LEU
1	C	301	LEU
1	D	433	LEU
1	B	400	LEU
1	B	456	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	331	HIS
1	B	333	HIS
1	C	306	ASN
1	B	288	HIS
1	B	297	GLN

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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	9CR	B	501	-	19,22,22	3.03	8 (42%)	26,30,30	3.89	18 (69%)
2	9CR	C	502	-	19,22,22	3.06	9 (47%)	26,30,30	3.50	18 (69%)

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	9CR	B	501	-	-	0/13/32/32	0/1/1/1
2	9CR	C	502	-	-	0/13/32/32	0/1/1/1

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	9CR	C12-C13	-5.35	1.34	1.45
2	C	502	9CR	C12-C13	-5.05	1.34	1.45
2	C	502	9CR	C8-C9	-4.10	1.36	1.45
2	B	501	9CR	C8-C9	-3.80	1.37	1.45
2	B	501	9CR	C11-C10	-3.20	1.34	1.43

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	502	9CR	C1-C6-C5	-5.54	115.08	122.50
2	B	501	9CR	C1-C6-C5	-5.48	115.17	122.50
2	B	501	9CR	C18-C5-C6	-4.51	119.82	124.62
2	B	501	9CR	C8-C9-C10	-4.10	112.35	118.95
2	C	502	9CR	C18-C5-C4	-3.40	106.89	113.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	9CR	14	0
2	C	502	9CR	5	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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.