wwPDB X-ray Structure Validation Summary Report (i)

Apr 30, 2025 – 08:08 PM JST

PDB ID	:	9IWJ / pdb_00009iwj
Title	:	X-ray structure of human PPARalpha ligand binding domain-NCoR2 corepressor peptide co-crystals obtained by co-crystallization
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Deposited on	:	2024-07-25
Resolution	:	2.48 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

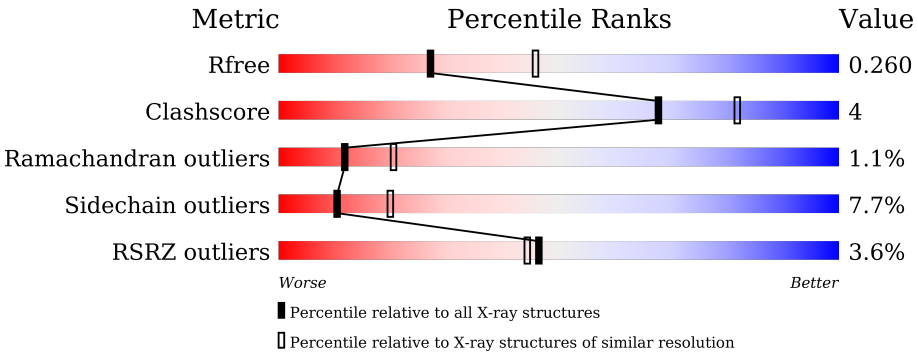
MolProbity	:	4-5-2 with Phenix2.0rc1
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 2.48 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}	164625	7106 (2.50-2.46)
Clashscore	180529	7991 (2.50-2.46)
Ramachandran outliers	177936	7888 (2.50-2.46)
Sidechain outliers	177891	7890 (2.50-2.46)
RSRZ outliers	164620	7106 (2.50-2.46)

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 of 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 <=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	273	3% 72% 8% • 19%
1	B	273	3% 69% 11% • 18%
1	C	273	4% 68% 12% • 18%
1	D	273	2% 70% 13% 16%
2	E	22	18% 45% 9% 9% 36%
2	F	22	50% 14% 36%

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Mol	Chain	Length	Quality of chain
2	G	22	
2	H	22	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7495 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 Peroxisome proliferator-activated receptor alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	0	0	0
			1746	1127	290	315	14			
1	B	225	Total	C	N	O	S	0	0	0
			1766	1138	292	322	14			
1	C	223	Total	C	N	O	S	0	1	0
			1756	1129	292	321	14			
1	D	228	Total	C	N	O	S	0	1	0
			1803	1160	300	328	15			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	196	GLY	-	expression tag	UNP Q07869
A	197	SER	-	expression tag	UNP Q07869
A	198	HIS	-	expression tag	UNP Q07869
A	199	MET	-	expression tag	UNP Q07869
B	196	GLY	-	expression tag	UNP Q07869
B	197	SER	-	expression tag	UNP Q07869
B	198	HIS	-	expression tag	UNP Q07869
B	199	MET	-	expression tag	UNP Q07869
C	196	GLY	-	expression tag	UNP Q07869
C	197	SER	-	expression tag	UNP Q07869
C	198	HIS	-	expression tag	UNP Q07869
C	199	MET	-	expression tag	UNP Q07869
D	196	GLY	-	expression tag	UNP Q07869
D	197	SER	-	expression tag	UNP Q07869
D	198	HIS	-	expression tag	UNP Q07869
D	199	MET	-	expression tag	UNP Q07869

- Molecule 2 is a protein called Nuclear receptor corepressor 2.

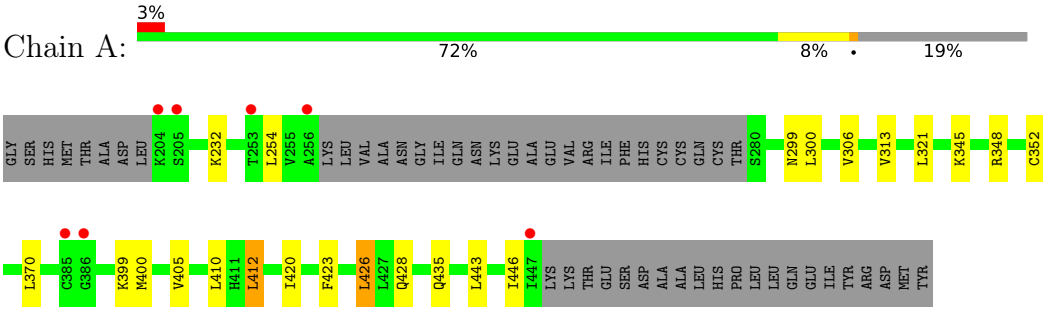
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	14	Total	C	N	O	S	0	0	0
			104	68	18	17	1			
2	F	14	Total	C	N	O	S	0	0	0
			108	71	19	17	1			
2	G	15	Total	C	N	O	S	0	0	0
			112	72	19	20	1			
2	H	13	Total	C	N	O	S	0	0	0
			100	66	17	16	1			

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

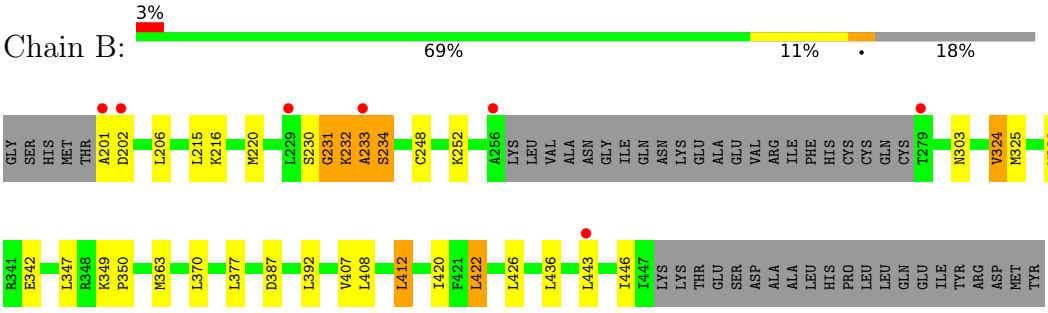
• Molecule 1: Peroxisome proliferator-activated receptor alpha

Chain A:



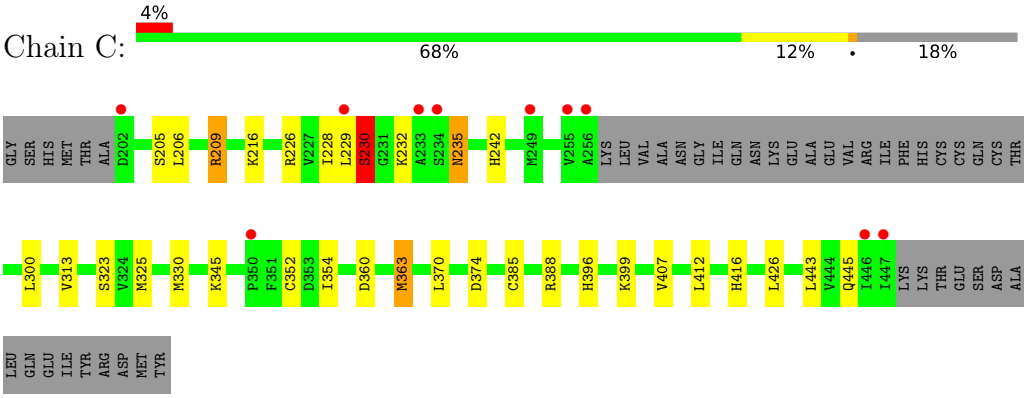
• Molecule 1: Peroxisome proliferator-activated receptor alpha

Chain B:



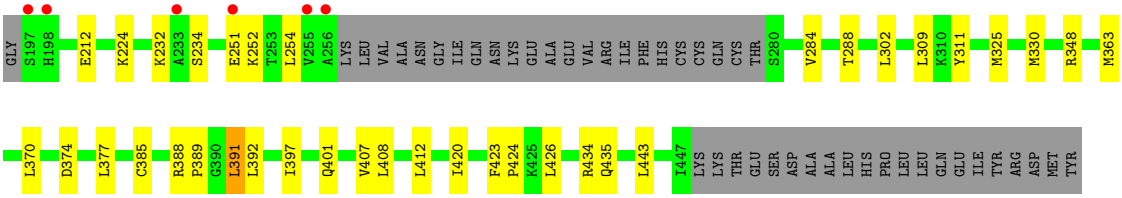
• Molecule 1: Peroxisome proliferator-activated receptor alpha

Chain C:



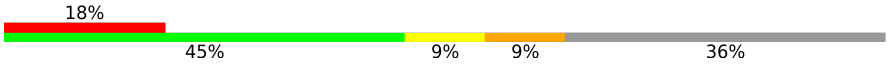
• Molecule 1: Peroxisome proliferator-activated receptor alpha

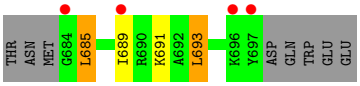
Chain D:



• Molecule 2: Nuclear receptor corepressor 2

Chain E:



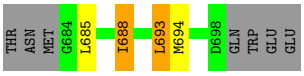


• Molecule 2: Nuclear receptor corepressor 2

Chain F:

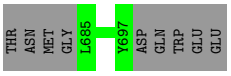
• Molecule 2: Nuclear receptor corepressor 2

Chain G:



• Molecule 2: Nuclear receptor corepressor 2

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	99.73Å 112.15Å 122.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.71 – 2.48 38.71 – 2.48	Depositor EDS
% Data completeness (in resolution range)	99.9 (38.71-2.48) 99.9 (38.71-2.48)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.17 (at 2.48Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575-000)	Depositor
R, R_{free}	0.225 , 0.254 0.234 , 0.260	Depositor DCC
R_{free} test set	2558 reflections (5.17%)	wwPDB-VP
Wilson B-factor (Å^2)	56.1	Xtriage
Anisotropy	0.282	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 31.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7495	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.77% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.10	0/1777	0.26	0/2395
1	B	0.11	0/1797	0.32	0/2426
1	C	0.10	0/1787	0.29	0/2412
1	D	0.11	0/1835	0.29	0/2475
2	E	0.10	0/104	0.28	0/137
2	F	0.08	0/108	0.26	0/141
2	G	0.11	0/112	0.29	0/148
2	H	0.13	0/100	0.41	0/132
All	All	0.11	0/7620	0.29	0/10266

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	C	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	230	SER	Peptide
1	C	232	LYS	Peptide

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	1746	0	1790	9	0
1	B	1766	0	1795	11	0
1	C	1756	0	1770	18	0
1	D	1803	0	1834	12	0
2	E	104	0	111	4	0
2	F	108	0	122	1	0
2	G	112	0	115	4	0
2	H	100	0	108	0	0
All	All	7495	0	7645	53	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 4.

The worst 5 of 53 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:231:GLY:O	1:B:233:ALA:N	2.25	0.68
1:B:412:LEU:HD21	1:B:426:LEU:HD12	1.77	0.66
1:B:324:VAL:HG22	1:B:331:LEU:HB2	1.78	0.66
1:A:313:VAL:HG11	2:E:685:LEU:HD11	1.78	0.64
1:B:340:THR:HG22	1:B:342:GLU:H	1.63	0.63

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	217/273 (80%)	211 (97%)	5 (2%)	1 (0%)	25 41
1	B	221/273 (81%)	208 (94%)	8 (4%)	5 (2%)	5 7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	220/273 (81%)	214 (97%)	4 (2%)	2 (1%)	14 26
1	D	225/273 (82%)	217 (96%)	6 (3%)	2 (1%)	14 26
2	E	12/22 (54%)	11 (92%)	1 (8%)	0	100 100
2	F	12/22 (54%)	12 (100%)	0	0	100 100
2	G	13/22 (59%)	13 (100%)	0	0	100 100
2	H	11/22 (50%)	9 (82%)	2 (18%)	0	100 100
All	All	931/1180 (79%)	895 (96%)	26 (3%)	10 (1%)	12 20

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	234	SER
1	B	231	GLY
1	D	252	LYS
1	D	348	ARG
1	C	229	LEU

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	193/238 (81%)	180 (93%)	13 (7%)	13 25
1	B	194/238 (82%)	175 (90%)	19 (10%)	6 12
1	C	192/238 (81%)	182 (95%)	10 (5%)	19 37
1	D	199/238 (84%)	185 (93%)	14 (7%)	12 23
2	E	9/18 (50%)	6 (67%)	3 (33%)	0 0
2	F	10/18 (56%)	8 (80%)	2 (20%)	1 1
2	G	10/18 (56%)	8 (80%)	2 (20%)	1 1
2	H	9/18 (50%)	9 (100%)	0	100 100
All	All	816/1024 (80%)	753 (92%)	63 (8%)	10 20

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	420	ILE
1	D	443	LEU
1	C	235	ASN
1	D	435	GLN
2	F	693	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	219	ASN
1	D	336	ASN
1	D	406	HIS
1	D	401	GLN
1	B	415	ASN

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 oligosaccharides 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

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, 95^{th} 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	221/273 (80%)	0.32	7 (3%) 50 48	46, 68, 92, 110	0
1	B	225/273 (82%)	0.14	7 (3%) 51 49	37, 53, 89, 110	0
1	C	223/273 (81%)	0.39	10 (4%) 39 36	29, 66, 99, 113	1 (0%)
1	D	228/273 (83%)	0.07	6 (2%) 57 55	26, 50, 88, 100	1 (0%)
2	E	14/22 (63%)	1.40	4 (28%) 1 1	76, 85, 93, 94	0
2	F	14/22 (63%)	0.12	0 100 100	49, 60, 72, 74	0
2	G	15/22 (68%)	0.82	0 100 100	70, 80, 89, 110	0
2	H	13/22 (59%)	0.65	0 100 100	51, 64, 83, 84	0
All	All	953/1180 (80%)	0.26	34 (3%) 46 44	26, 61, 93, 113	2 (0%)

The worst 5 of 34 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	256	ALA	4.4
1	B	279	THR	4.1
1	D	233	ALA	3.7
1	A	447	ILE	3.4
1	D	256	ALA	3.4

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 monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.