



wwPDB X-ray Structure Validation Summary Report ⓘ

May 7, 2026 – 10:34 AM EDT

PDB ID : 2GL8 / pdb_00002gl8
Title : Human Retinoic acid receptor RXR-gamma ligand-binding domain
Authors : Min, J.R.; Schuetz, A.; Loppnau, P.; Weigelt, J.; Sundstrom, M.; Arrowsmith, C.H.; Edwards, A.M.; Bochkarev, A.; Plotnikov, A.N.; Structural Genomics Consortium (SGC)
Deposited on : 2006-04-04
Resolution : 2.40 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

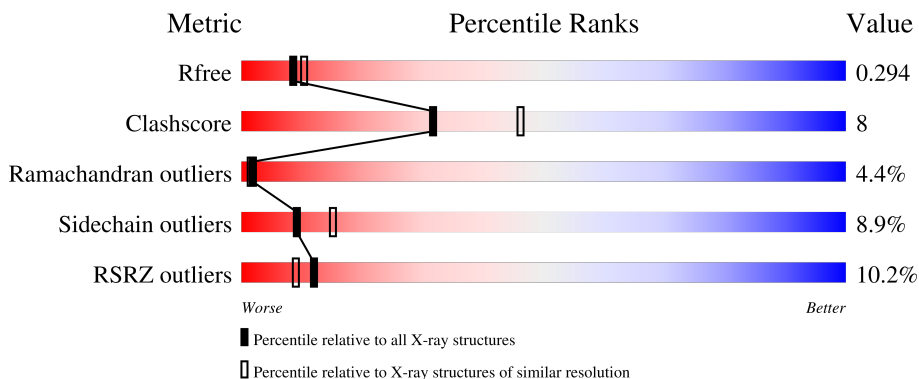
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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 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 $\leq 5\%$. 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	241	 8% 54% 19% 6% 21%
1	B	241	 5% 59% 19% 20%
1	C	241	 9% 63% 14% 20%
1	D	241	 11% 65% 13% 19%

2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 5916 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-gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	190	1459	931	254	268	6	0	0	0
1	B	192	1454	928	257	263	6	0	0	0
1	C	194	1447	919	256	266	6	0	0	0
1	D	195	1451	920	254	271	6	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	cloning artifact	UNP P48443
A	2	SER	-	cloning artifact	UNP P48443
A	3	HIS	-	cloning artifact	UNP P48443
A	4	ASN	-	cloning artifact	UNP P48443
B	1	GLY	-	cloning artifact	UNP P48443
B	2	SER	-	cloning artifact	UNP P48443
B	3	HIS	-	cloning artifact	UNP P48443
B	4	ASN	-	cloning artifact	UNP P48443
C	1	GLY	-	cloning artifact	UNP P48443
C	2	SER	-	cloning artifact	UNP P48443
C	3	HIS	-	cloning artifact	UNP P48443
C	4	ASN	-	cloning artifact	UNP P48443
D	1	GLY	-	cloning artifact	UNP P48443
D	2	SER	-	cloning artifact	UNP P48443
D	3	HIS	-	cloning artifact	UNP P48443
D	4	ASN	-	cloning artifact	UNP P48443

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	32	Total O 32 32	0	0
2	B	23	Total O 23 23	0	0
2	C	27	Total O 27 27	0	0
2	D	23	Total O 23 23	0	0

LEU
GLN
ILE
THR

● Molecule 1: Retinoic acid receptor RXR-gamma

Chain D:  11% 65% 13% 19%

GLY SER HIS ASN ALA THR SER GLY HIS GLU D11 M12 P13 V14 L18 V24 E25 P26 LYS THR GLU SER TYR GLY ASP MET MET MET ASN GLU ASN SER THR THR ASN ASP ASP PRO VAL THR ASN ILE CYS HIS A50 A51 D52 K53 Q54 V59 T72 D75 L80 R81 W84 N85

L88 F92 V99 Q100 A106 T107 G108 L109 I124 E131 M141 L146 L149 R150 A151 K160 K174 T178 S206 I207 G208 L209 K210 C211 L212 E213 H214 L215 F216 F217 F218 F219 L220 I221 G222 T224 F225 D226 D227 T228 PHE LEU MET MET LEU

GLU
THR
PRO
LEU
GLN
ILE
THR

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	48.07Å 161.32Å 68.68Å 90.00° 109.50° 90.00°	Depositor
Resolution (Å)	80.58 – 2.40 80.58 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.0 (80.58-2.40) 99.0 (80.58-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.39Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.243 , 0.296 0.242 , 0.294	Depositor DCC
R_{free} test set	1936 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	68.9	Xtrriage
Anisotropy	0.026	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 84.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.031 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5916	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.85% 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	0.84	2/1484 (0.1%)	1.12	6/2005 (0.3%)
1	B	0.91	3/1480 (0.2%)	1.03	3/2001 (0.1%)
1	C	0.73	1/1473 (0.1%)	1.04	4/1989 (0.2%)
1	D	0.65	0/1475	1.05	3/1996 (0.2%)
All	All	0.79	6/5912 (0.1%)	1.06	16/7991 (0.2%)

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	A	0	1
1	B	0	2
1	D	0	1
All	All	0	4

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	226	ILE	C-O	17.39	1.58	1.23
1	C	26	PRO	C-O	9.17	1.41	1.23
1	A	224	THR	C-O	8.91	1.41	1.23
1	B	212	LEU	C-O	8.32	1.33	1.24
1	B	212	LEU	CG-CD2	5.65	1.71	1.52

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	225	PRO	N-CA-CB	9.59	113.15	102.60
1	A	224	THR	CA-C-O	-6.57	109.63	120.80
1	A	99	VAL	N-CA-C	5.73	117.45	109.55
1	B	217	PHE	N-CA-C	5.65	117.65	109.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	223	ASP	N-CA-C	5.65	117.64	108.26

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	214	HIS	Peptide
1	B	53	LYS	Peptide
1	B	54	GLN	Peptide
1	D	223	ASP	Peptide

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	1459	0	1470	39	0
1	B	1454	0	1454	20	0
1	C	1447	0	1434	18	0
1	D	1451	0	1424	20	0
2	A	32	0	0	0	0
2	B	23	0	0	0	0
2	C	27	0	0	0	0
2	D	23	0	0	0	0
All	All	5916	0	5782	94	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 94 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:215:LEU:HG	1:B:216:PHE:H	1.35	0.89
1:A:94:HIS:HD2	1:A:141:MET:HE2	1.40	0.86
1:A:219:LYS:HA	1:A:220:LEU:HB2	1.57	0.84
1:A:219:LYS:HA	1:A:220:LEU:CB	2.16	0.76
1:A:72:THR:HG22	1:A:75:ASP:H	1.51	0.76

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	186/241 (77%)	169 (91%)	9 (5%)	8 (4%)	2	1
1	B	188/241 (78%)	168 (89%)	13 (7%)	7 (4%)	2	2
1	C	190/241 (79%)	170 (90%)	8 (4%)	12 (6%)	1	0
1	D	191/241 (79%)	178 (93%)	7 (4%)	6 (3%)	3	3
All	All	755/964 (78%)	685 (91%)	37 (5%)	33 (4%)	2	1

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	100	GLN
1	A	218	PHE
1	A	220	LEU
1	B	51	ALA
1	B	53	LYS

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	155/211 (74%)	140 (90%)	15 (10%)	8	12
1	B	151/211 (72%)	134 (89%)	17 (11%)	5	8
1	C	150/211 (71%)	139 (93%)	11 (7%)	13	22

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	149/211 (71%)	138 (93%)	11 (7%)	13	22
All	All	605/844 (72%)	551 (91%)	54 (9%)	9	15

5 of 54 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	183	THR
1	C	25	GLU
1	D	160	LYS
1	B	210	LYS
1	C	11	ASP

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	C	85	ASN
1	C	117	HIS
1	D	112	HIS
1	C	156	ASN
1	B	117	HIS

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 [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	190/241 (78%)	0.52	19 (10%) 12 9	41, 54, 74, 86	0
1	B	192/241 (79%)	0.51	13 (6%) 23 20	44, 63, 84, 87	0
1	C	194/241 (80%)	0.68	21 (10%) 11 8	43, 62, 75, 78	0
1	D	195/241 (80%)	0.78	26 (13%) 7 5	45, 69, 90, 95	0
All	All	771/964 (79%)	0.62	79 (10%) 12 9	41, 62, 85, 95	0

The worst 5 of 79 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	106	ALA	6.6
1	C	55	LEU	5.7
1	A	224	THR	5.5
1	B	226	ILE	4.7
1	B	216	PHE	4.5

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 oligosaccharides 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.