



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 3, 2016 – 04:35 PM EDT

PDB ID : 1XLS  
Title : Crystal structure of the mouse CAR/RXR LBD heterodimer bound to TCPOBOP and 9cRA and a TIF2 peptide containing the third LXXLL motifs  
Authors : Suino, K.; peng, L.; Reynolds, R.; Li, Y.; Cha, J.-Y.; Repa, J.J.; Kliewer, S.A.; Xu, H.E.  
Deposited on : 2004-09-30  
Resolution : 2.96 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028320
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)	:	rb-20028320



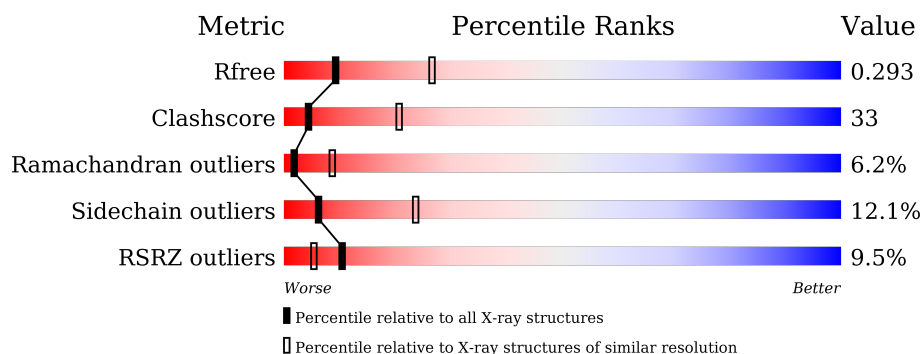
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.96 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	2184 (3.00-2.92)
Clashscore	102246	2552 (3.00-2.92)
Ramachandran outliers	100387	2468 (3.00-2.92)
Sidechain outliers	100360	2471 (3.00-2.92)
RSRZ outliers	91569	2201 (3.00-2.92)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	232	<div> <div>10%</div> <div>56%</div> <div>35%</div> <div>8%</div> </div>
1	B	232	<div> <div>11%</div> <div>55%</div> <div>37%</div> <div>8%</div> </div>
1	C	232	<div> <div>11%</div> <div>57%</div> <div>34%</div> <div>9%</div> </div>
1	D	232	<div> <div>9%</div> <div>56%</div> <div>34%</div> <div>9%</div> </div>
2	E	242	<div> <div>5%</div> <div>44%</div> <div>43%</div> <div>10%</div> <div>.</div> </div>
2	F	242	<div> <div>6%</div> <div>47%</div> <div>42%</div> <div>9%</div> <div>.</div> </div>

Continued on next page...



Continued from previous page...

Mol	Chain	Length	Quality of chain
2	G	242	
2	H	242	
3	I	18	
3	J	18	
3	K	18	
3	L	18	
3	M	18	
3	N	18	
3	O	18	
3	P	18	

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
4	9CR	A	801	-	-	-	X
4	9CR	D	804	-	-	-	X
5	TCD	E	805	-	-	-	X
5	TCD	H	808	-	-	-	X



## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16288 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	232	Total	C	N	O	S	0	0	0
			1755	1117	306	322	10			
1	B	232	Total	C	N	O	S	0	0	0
			1755	1117	306	322	10			
1	C	232	Total	C	N	O	S	0	0	0
			1755	1117	306	322	10			
1	D	232	Total	C	N	O	S	0	0	0
			1755	1117	306	322	10			

- Molecule 2 is a protein called Orphan nuclear receptor NR1I3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	242	Total	C	N	O	S	0	0	0
			1969	1269	334	353	13			
2	F	242	Total	C	N	O	S	0	0	0
			1969	1269	334	353	13			
2	G	242	Total	C	N	O	S	0	0	0
			1969	1269	334	353	13			
2	H	242	Total	C	N	O	S	0	0	0
			1969	1269	334	353	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	146	ARG	LYS	CONFLICT	UNP O35627
F	146	ARG	LYS	CONFLICT	UNP O35627
G	146	ARG	LYS	CONFLICT	UNP O35627
H	146	ARG	LYS	CONFLICT	UNP O35627

- Molecule 3 is a protein called Nuclear receptor coactivator 2.



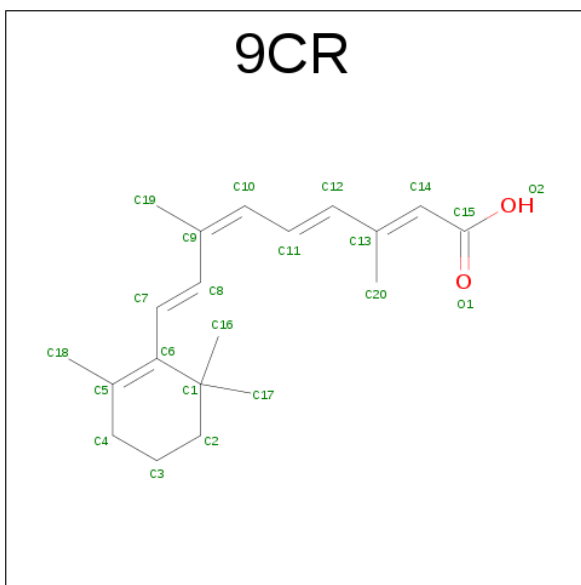
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	16	Total	C	N	O	0	0	0
			131	82	22	27			
3	J	16	Total	C	N	O	0	0	0
			131	82	22	27			
3	K	16	Total	C	N	O	0	0	0
			131	82	22	27			
3	L	16	Total	C	N	O	0	0	0
			131	82	22	27			
3	M	18	Total	C	N	O	0	0	0
			149	92	25	32			
3	N	18	Total	C	N	O	0	0	0
			149	92	25	32			
3	O	18	Total	C	N	O	0	0	0
			149	92	25	32			
3	P	18	Total	C	N	O	0	0	0
			149	92	25	32			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	739	ALA	LYS	CONFLICT	UNP Q9WUI9
J	739	ALA	LYS	CONFLICT	UNP Q9WUI9
K	739	ALA	LYS	CONFLICT	UNP Q9WUI9
L	739	ALA	LYS	CONFLICT	UNP Q9WUI9
M	739	ALA	LYS	CONFLICT	UNP Q9WUI9
N	739	ALA	LYS	CONFLICT	UNP Q9WUI9
O	739	ALA	LYS	CONFLICT	UNP Q9WUI9
P	739	ALA	LYS	CONFLICT	UNP Q9WUI9

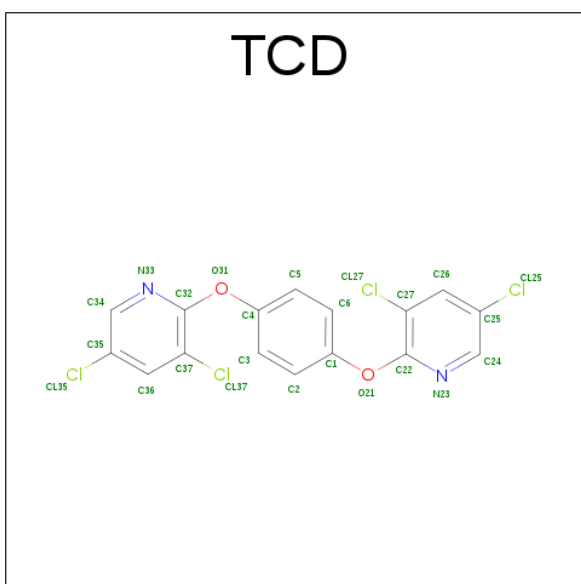
- Molecule 4 is (9CIS)-RETINOIC ACID (three-letter code: 9CR) (formula: C<sub>20</sub>H<sub>28</sub>O<sub>2</sub>).





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

- Molecule 5 is 3,5-DICHLORO-2-{4-[(3,5-DICHLOROPYRIDIN-2-YL)OXY]PHENOXY}PYRIDINE (three-letter code: TCD) (formula:  $C_{16}H_8Cl_4N_2O_2$ ).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	E	1	Total	C	Cl	N	O	0	0
			24	16	4	2	2		
5	F	1	Total	C	Cl	N	O	0	0
			24	16	4	2	2		
5	G	1	Total	C	Cl	N	O	0	0
			24	16	4	2	2		
5	H	1	Total	C	Cl	N	O	0	0
			24	16	4	2	2		

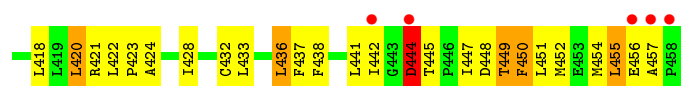
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	7	Total	O	0	0
			7	7		
6	B	8	Total	O	0	0
			8	8		
6	C	10	Total	O	0	0
			10	10		
6	D	20	Total	O	0	0
			20	20		
6	E	4	Total	O	0	0
			4	4		
6	F	17	Total	O	0	0
			17	17		
6	G	10	Total	O	0	0
			10	10		
6	H	4	Total	O	0	0
			4	4		
6	I	1	Total	O	0	0
			1	1		
6	J	1	Total	O	0	0
			1	1		
6	K	1	Total	O	0	0
			1	1		
6	L	1	Total	O	0	0
			1	1		
6	M	1	Total	O	0	0
			1	1		
6	O	1	Total	O	0	0
			1	1		
6	P	2	Total	O	0	0
			2	2		

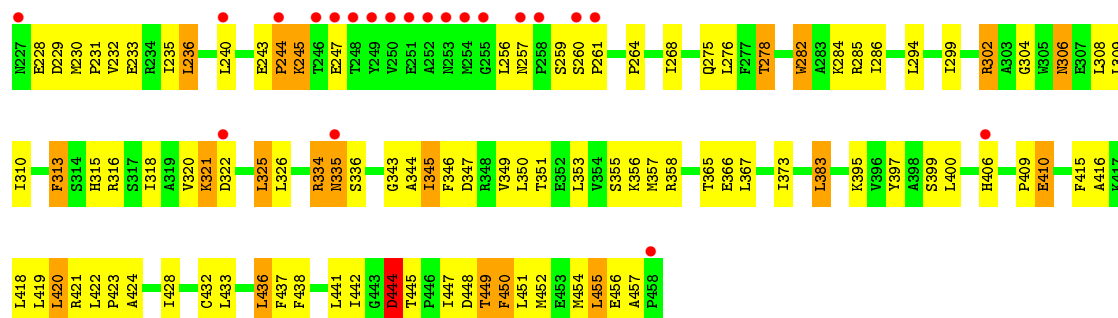




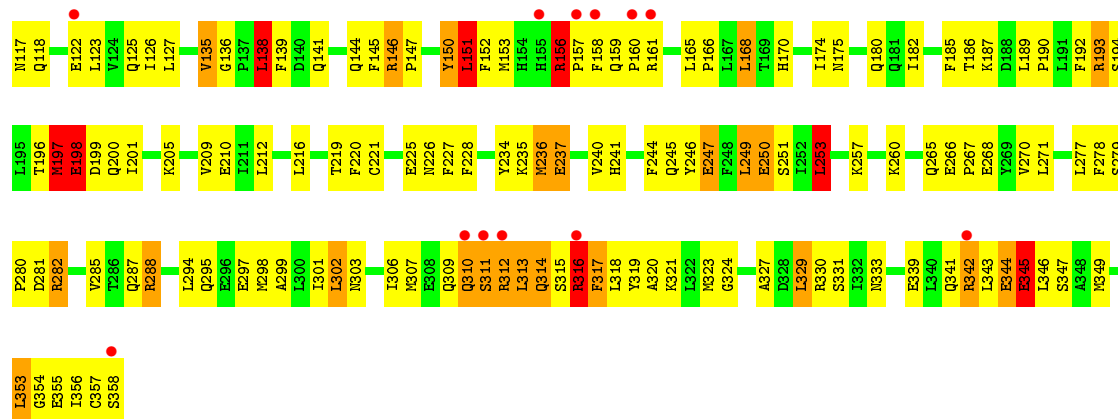
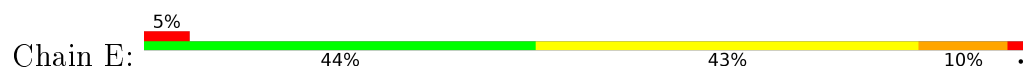




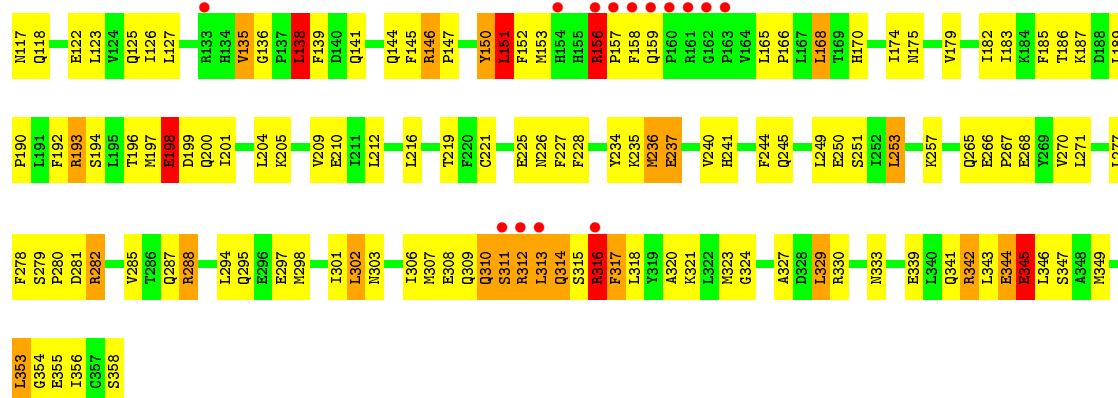
• Molecule 1: Retinoic acid receptor RXR-alpha



• Molecule 2: Orphan nuclear receptor NR1I3

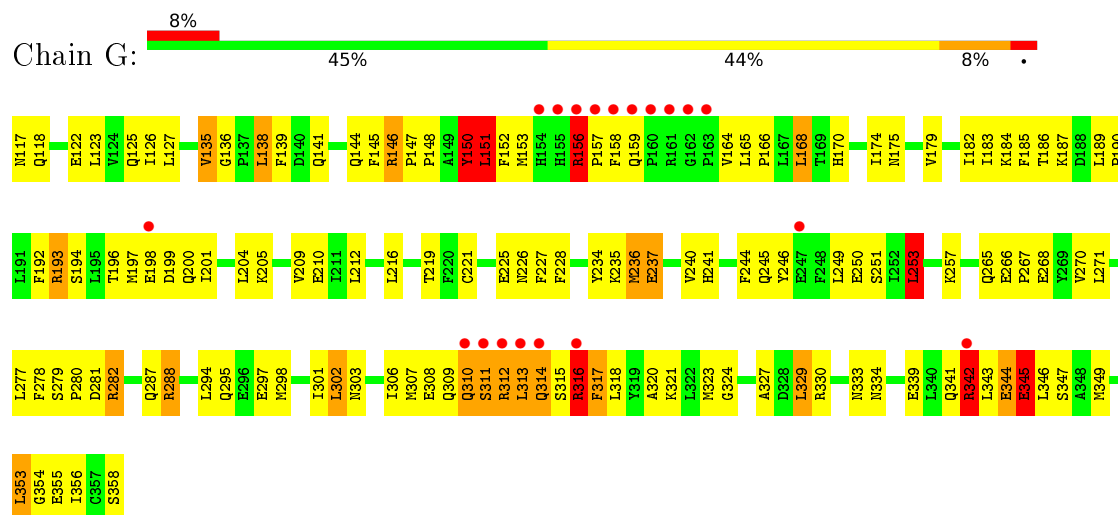


• Molecule 2: Orphan nuclear receptor NR1I3

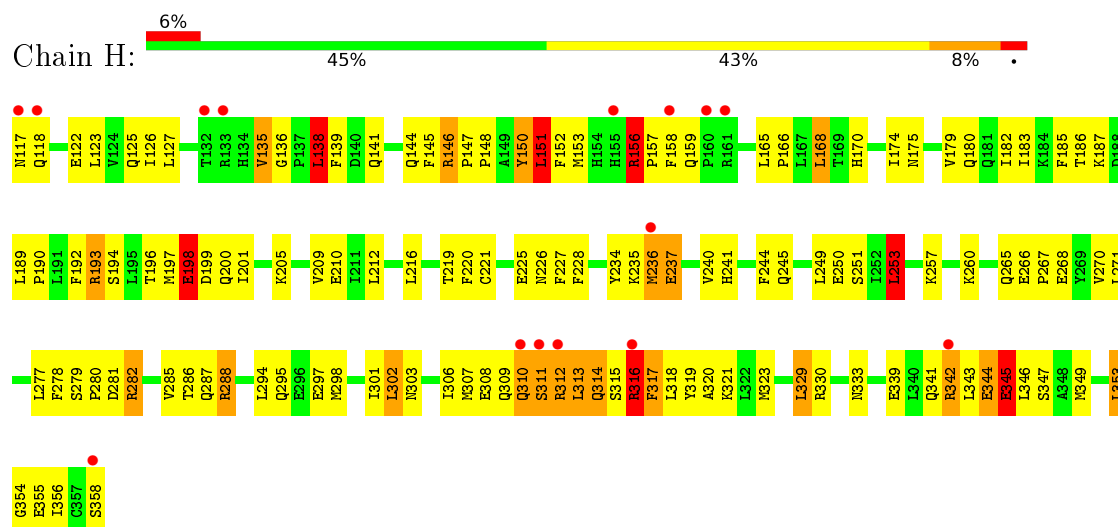




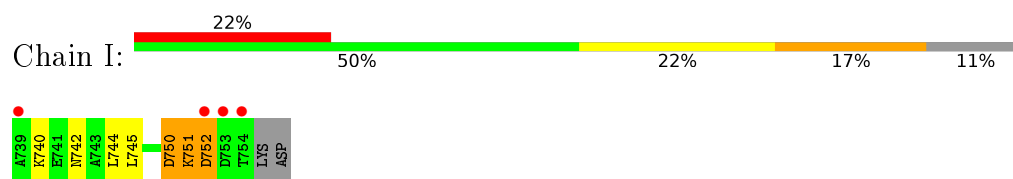
- Molecule 2: Orphan nuclear receptor NR1I3



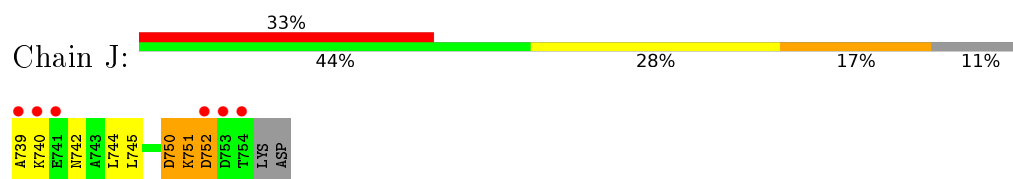
- Molecule 2: Orphan nuclear receptor NR1I3



- Molecule 3: Nuclear receptor coactivator 2

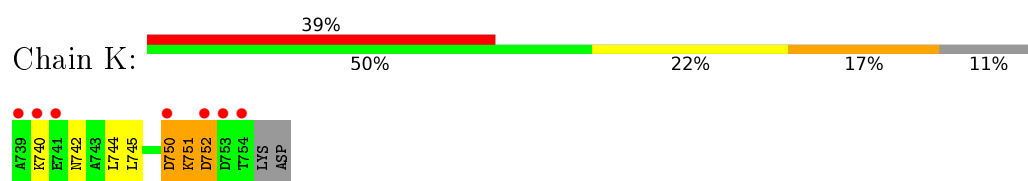


- Molecule 3: Nuclear receptor coactivator 2



- Molecule 3: Nuclear receptor coactivator 2

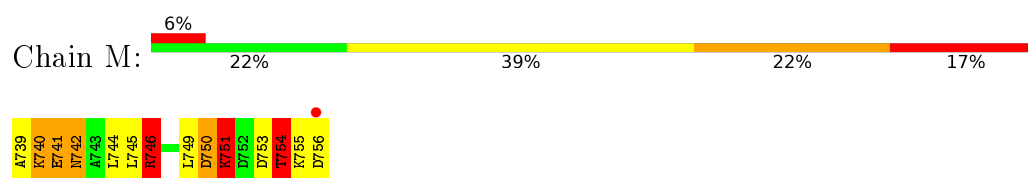




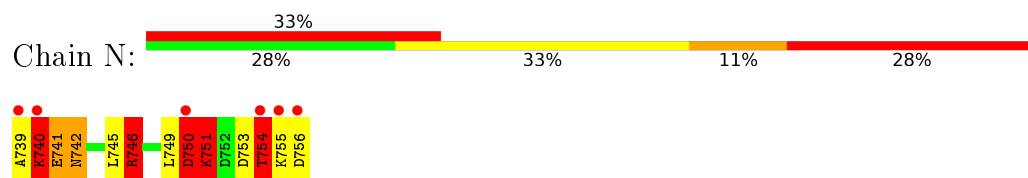
- Molecule 3: Nuclear receptor coactivator 2



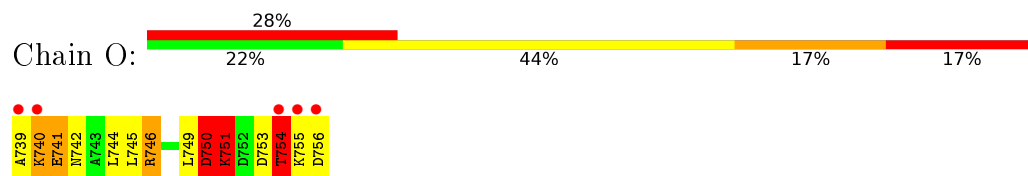
- Molecule 3: Nuclear receptor coactivator 2



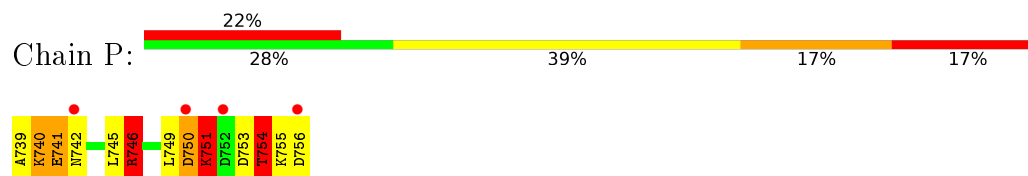
- Molecule 3: Nuclear receptor coactivator 2



- Molecule 3: Nuclear receptor coactivator 2



- Molecule 3: Nuclear receptor coactivator 2





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.27Å 88.38Å 105.49Å 79.02° 85.81° 67.22°	Depositor
Resolution (Å)	19.99 – 2.96 19.99 – 2.97	Depositor EDS
% Data completeness (in resolution range)	92.5 (19.99-2.96) 86.7 (19.99-2.97)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.12 (at 2.98Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.255 , 0.303 0.250 , 0.293	Depositor DCC
$R_{free}$ test set	3463 reflections (8.12%)	DCC
Wilson B-factor (Å <sup>2</sup> )	56.2	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 57.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	16288	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 ⓘ

### 5.1 Standard geometry ⓘ

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

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	0.40	0/1790	0.60	0/2414
1	B	0.41	0/1790	0.61	0/2414
1	C	0.40	0/1790	0.60	0/2414
1	D	0.40	0/1790	0.61	0/2414
2	E	0.48	0/2016	0.94	16/2727 (0.6%)
2	F	0.48	1/2016 (0.0%)	0.85	8/2727 (0.3%)
2	G	0.48	2/2016 (0.1%)	0.83	6/2727 (0.2%)
2	H	0.54	1/2016 (0.0%)	1.28	14/2727 (0.5%)
3	I	0.39	0/131	0.60	0/175
3	J	0.40	0/131	0.62	0/175
3	K	0.34	0/131	0.61	0/175
3	L	0.39	0/131	0.60	0/175
3	M	1.01	1/149 (0.7%)	3.00	7/197 (3.6%)
3	N	0.84	1/149 (0.7%)	1.92	7/197 (3.6%)
3	O	0.84	1/149 (0.7%)	3.56	10/197 (5.1%)
3	P	0.99	1/149 (0.7%)	2.16	8/197 (4.1%)
All	All	0.48	8/16344 (0.0%)	0.96	76/22052 (0.3%)

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
2	G	0	1
3	M	0	1
3	N	0	1
3	P	0	1
All	All	0	4

The worst 5 of 8 bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	193	ARG	CZ-NH1	-12.28	1.17	1.33
3	M	750	ASP	CB-CG	-7.52	1.35	1.51
3	P	750	ASP	CB-CG	-7.52	1.35	1.51
2	G	342	ARG	CB-CG	-6.12	1.36	1.52
3	N	750	ASP	CB-CG	-5.28	1.40	1.51

The worst 5 of 76 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	193	ARG	NE-CZ-NH2	33.36	136.98	120.30
3	O	746	ARG	NE-CZ-NH1	-30.74	104.93	120.30
3	O	746	ARG	NE-CZ-NH2	27.55	134.08	120.30
3	M	746	ARG	NE-CZ-NH1	-26.46	107.07	120.30
2	H	342	ARG	NE-CZ-NH1	-24.98	107.81	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	G	150	TYR	Sidechain
3	M	746	ARG	Sidechain
3	N	746	ARG	Sidechain
3	P	746	ARG	Sidechain

## 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	1755	0	1733	116	0
1	B	1755	0	1733	112	1
1	C	1755	0	1733	89	0
1	D	1755	0	1733	90	0
2	E	1969	0	1964	164	1
2	F	1969	0	1964	140	2
2	G	1969	0	1964	165	0
2	H	1969	0	1964	156	2
3	I	131	0	132	9	0
3	J	131	0	132	11	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	K	131	0	132	9	0
3	L	131	0	132	10	0
3	M	149	0	149	29	0
3	N	149	0	149	27	0
3	O	149	0	149	28	0
3	P	149	0	149	34	0
4	A	22	0	27	3	0
4	B	22	0	27	3	0
4	C	22	0	27	4	0
4	D	22	0	27	4	0
5	E	24	0	8	1	0
5	F	24	0	8	1	0
5	G	24	0	8	1	0
5	H	24	0	8	1	0
6	A	7	0	0	1	0
6	B	8	0	0	1	0
6	C	10	0	0	1	0
6	D	20	0	0	1	0
6	E	4	0	0	2	0
6	F	17	0	0	2	0
6	G	10	0	0	1	0
6	H	4	0	0	0	0
6	I	1	0	0	0	0
6	J	1	0	0	3	0
6	K	1	0	0	0	0
6	L	1	0	0	1	0
6	M	1	0	0	0	0
6	O	1	0	0	0	0
6	P	2	0	0	1	0
All	All	16288	0	16052	1058	3

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 33.

The worst 5 of 1058 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)
2:E:157:PRO:CD	2:G:342:ARG:HH12	1.16	1.54
2:E:157:PRO:CD	2:G:342:ARG:NH1	1.74	1.39
2:E:157:PRO:HD3	2:G:342:ARG:NH1	1.09	1.37
1:A:406:HIS:CD2	1:B:233:GLU:HA	1.64	1.32

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:HIS:CE1	1:B:236:LEU:HB3	1.72	1.25

All (3) 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)
2:F:342:ARG:NH1	2:H:156:ARG:O[1_655]	1.81	0.39
2:F:342:ARG:NH1	2:H:157:PRO:CD[1_655]	1.88	0.32
1:B:442:ILE:O	2:E:161:ARG:NH1[1_554]	2.17	0.03

## 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	230/232 (99%)	191 (83%)	26 (11%)	13 (6%)	2	10
1	B	230/232 (99%)	190 (83%)	27 (12%)	13 (6%)	2	10
1	C	230/232 (99%)	191 (83%)	25 (11%)	14 (6%)	2	9
1	D	230/232 (99%)	189 (82%)	27 (12%)	14 (6%)	2	9
2	E	240/242 (99%)	206 (86%)	22 (9%)	12 (5%)	3	13
2	F	240/242 (99%)	207 (86%)	20 (8%)	13 (5%)	2	11
2	G	240/242 (99%)	206 (86%)	21 (9%)	13 (5%)	2	11
2	H	240/242 (99%)	209 (87%)	18 (8%)	13 (5%)	2	11
3	I	14/18 (78%)	10 (71%)	3 (21%)	1 (7%)	1	6
3	J	14/18 (78%)	10 (71%)	3 (21%)	1 (7%)	1	6
3	K	14/18 (78%)	10 (71%)	3 (21%)	1 (7%)	1	6
3	L	14/18 (78%)	10 (71%)	3 (21%)	1 (7%)	1	6
3	M	16/18 (89%)	9 (56%)	3 (19%)	4 (25%)	0	0

Continued on next page...



*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	N	16/18 (89%)	10 (62%)	1 (6%)	5 (31%)	0	0
3	O	16/18 (89%)	10 (62%)	3 (19%)	3 (19%)	0	0
3	P	16/18 (89%)	9 (56%)	4 (25%)	3 (19%)	0	0
All	All	2000/2040 (98%)	1667 (83%)	209 (10%)	124 (6%)	2	9

5 of 124 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	244	PRO
1	A	245	LYS
1	A	256	LEU
1	A	260	SER
1	A	261	PRO

### 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	182/200 (91%)	163 (90%)	19 (10%)	9	30
1	B	182/200 (91%)	163 (90%)	19 (10%)	9	30
1	C	182/200 (91%)	163 (90%)	19 (10%)	9	30
1	D	182/200 (91%)	163 (90%)	19 (10%)	9	30
2	E	217/217 (100%)	191 (88%)	26 (12%)	6	24
2	F	217/217 (100%)	194 (89%)	23 (11%)	8	29
2	G	217/217 (100%)	193 (89%)	24 (11%)	8	27
2	H	217/217 (100%)	193 (89%)	24 (11%)	8	27
3	I	14/16 (88%)	10 (71%)	4 (29%)	0	2
3	J	14/16 (88%)	10 (71%)	4 (29%)	0	2
3	K	14/16 (88%)	10 (71%)	4 (29%)	0	2
3	L	14/16 (88%)	10 (71%)	4 (29%)	0	2
3	M	16/16 (100%)	11 (69%)	5 (31%)	0	1

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	N	16/16 (100%)	11 (69%)	5 (31%)	0	1
3	O	16/16 (100%)	11 (69%)	5 (31%)	0	1
3	P	16/16 (100%)	12 (75%)	4 (25%)	1	3
All	All	1716/1796 (96%)	1508 (88%)	208 (12%)	6	23

5 of 208 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	302	LEU
2	F	282	ARG
3	M	751	LYS
2	E	316	ARG
2	F	146	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 73 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	144	GLN
2	F	258	ASN
2	H	245	GLN
2	F	181	GLN
2	F	333	ASN

### 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

8 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
4	9CR	A	801	-	19,22,22	4.08	12 (63%)	26,30,30	2.92	15 (57%)
4	9CR	B	802	-	19,22,22	4.11	12 (63%)	26,30,30	2.93	15 (57%)
4	9CR	C	803	-	19,22,22	4.19	12 (63%)	26,30,30	2.95	15 (57%)
4	9CR	D	804	-	19,22,22	4.16	13 (68%)	26,30,30	2.92	14 (53%)
5	TCD	E	805	-	24,26,26	2.29	4 (16%)	24,36,36	1.63	6 (25%)
5	TCD	F	806	-	24,26,26	2.14	3 (12%)	24,36,36	1.39	3 (12%)
5	TCD	G	807	-	24,26,26	2.34	4 (16%)	24,36,36	1.58	5 (20%)
5	TCD	H	808	-	24,26,26	2.06	3 (12%)	24,36,36	1.45	4 (16%)

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
4	9CR	A	801	-	-	0/13/32/32	0/1/1/1
4	9CR	B	802	-	-	0/13/32/32	0/1/1/1
4	9CR	C	803	-	-	0/13/32/32	0/1/1/1
4	9CR	D	804	-	-	0/13/32/32	0/1/1/1
5	TCD	E	805	-	-	0/8/8/8	0/3/3/3
5	TCD	F	806	-	-	0/8/8/8	0/3/3/3
5	TCD	G	807	-	-	0/8/8/8	0/3/3/3
5	TCD	H	808	-	-	0/8/8/8	0/3/3/3

The worst 5 of 63 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	801	9CR	C4-C5	-4.61	1.41	1.51
4	D	804	9CR	C4-C5	-4.53	1.41	1.51

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	802	9CR	C4-C5	-4.50	1.41	1.51
4	C	803	9CR	C4-C5	-4.31	1.41	1.51
4	D	804	9CR	C3-C4	-3.59	1.40	1.52

The worst 5 of 77 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	801	9CR	C19-C9-C10	-5.76	114.52	122.89
4	D	804	9CR	C19-C9-C10	-5.75	114.52	122.89
4	C	803	9CR	C19-C9-C10	-5.73	114.56	122.89
4	B	802	9CR	C19-C9-C10	-5.73	114.56	122.89
4	B	802	9CR	C1-C6-C5	-5.56	115.06	122.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	801	9CR	3	0
4	B	802	9CR	3	0
4	C	803	9CR	4	0
4	D	804	9CR	4	0
5	E	805	TCD	1	0
5	F	806	TCD	1	0
5	G	807	TCD	1	0
5	H	808	TCD	1	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 ⓘ

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	232/232 (100%)	0.42	24 (10%) 9 4	22, 47, 126, 134	0
1	B	232/232 (100%)	0.54	25 (10%) 8 4	22, 50, 128, 137	0
1	C	232/232 (100%)	0.56	26 (11%) 7 4	21, 53, 127, 136	0
1	D	232/232 (100%)	0.43	21 (9%) 11 6	21, 50, 125, 135	0
2	E	242/242 (100%)	-0.04	12 (4%) 32 19	21, 44, 89, 122	0
2	F	242/242 (100%)	0.10	14 (5%) 26 14	16, 42, 89, 127	0
2	G	242/242 (100%)	0.15	19 (7%) 15 8	17, 44, 88, 126	0
2	H	242/242 (100%)	-0.01	15 (6%) 24 13	18, 44, 89, 121	0
3	I	16/18 (88%)	1.36	4 (25%) 1 1	43, 79, 130, 135	0
3	J	16/18 (88%)	2.41	6 (37%) 0 0	51, 82, 132, 134	0
3	K	16/18 (88%)	2.32	7 (43%) 0 0	53, 85, 134, 136	0
3	L	16/18 (88%)	1.25	5 (31%) 1 0	43, 77, 131, 137	0
3	M	18/18 (100%)	0.96	1 (5%) 28 15	37, 77, 121, 125	0
3	N	18/18 (100%)	1.66	6 (33%) 0 0	39, 76, 121, 129	0
3	O	18/18 (100%)	1.40	5 (27%) 1 0	39, 75, 120, 129	0
3	P	18/18 (100%)	0.94	4 (22%) 1 1	37, 80, 120, 124	0
All	All	2032/2040 (99%)	0.35	194 (9%) 10 5	16, 48, 120, 137	0

The worst 5 of 194 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	249	TYR	14.3
1	B	248	THR	14.0
1	C	255	GLY	12.3
3	K	754	THR	11.2
1	D	254	MET	10.7



## 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, 95<sup>th</sup> 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	TCD	E	805	24/24	0.81	0.30	4.96	27,42,54,54	0
4	9CR	A	801	22/22	0.92	0.39	3.53	31,43,48,53	0
4	9CR	D	804	22/22	0.93	0.33	3.09	31,39,44,49	0
5	TCD	H	808	24/24	0.82	0.27	3.03	27,37,54,54	0
4	9CR	C	803	22/22	0.86	0.26	1.36	32,41,48,48	0
4	9CR	B	802	22/22	0.90	0.27	1.18	26,36,41,47	0
5	TCD	G	807	24/24	0.89	0.22	0.92	12,38,54,54	0
5	TCD	F	806	24/24	0.92	0.19	0.28	14,35,54,54	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.