



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:37 AM GMT

PDB ID : 2HWR  
Title : Structural basis for the structure-activity relationships of Peroxisome Proliferator-Activated Receptor agonists  
Authors : Peng, Y.H.; Lu, I.L.; Mahindroo, N.; Lin, C.H.; Hsieh, H.P.; Wu, S.Y.  
Deposited on : 2006-08-01  
Resolution : 2.34 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

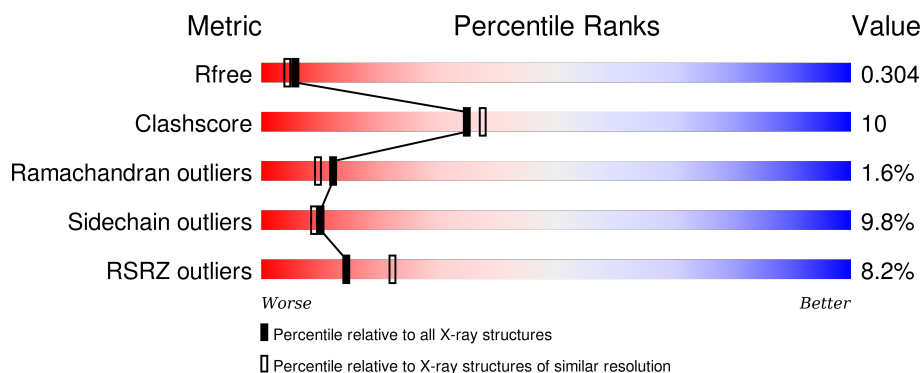
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.34 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	1406 (2.36-2.32)
Clashscore	102246	1509 (2.36-2.32)
Ramachandran outliers	100387	1490 (2.36-2.32)
Sidechain outliers	100360	1491 (2.36-2.32)
RSRZ outliers	91569	1412 (2.36-2.32)

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	271	
1	B	271	

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	DRD	A	101	-	-	-	X

## 2 Entry composition [i](#)

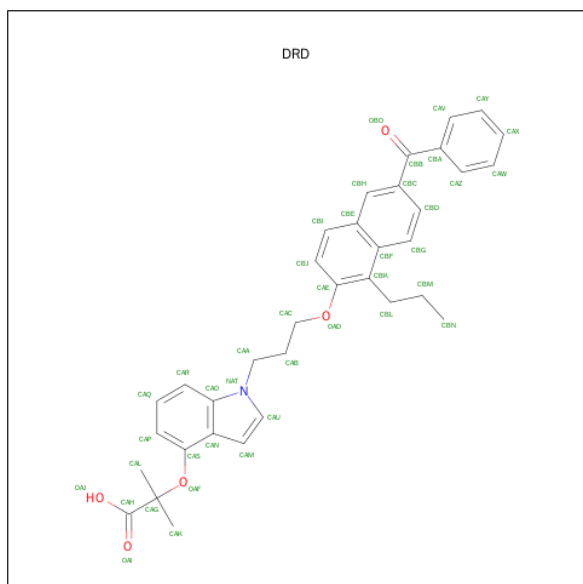
There are 3 unique types of molecules in this entry. The entry contains 4231 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	0	0	0
			2096	1355	340	391	10			
1	B	253	Total	C	N	O	S	0	0	0
			2017	1296	331	380	10			

- Molecule 2 is 2-[(1-{3-[(6-BENZOYL-1-PROPYL-2-NAPHTHYL)OXY]PROPYL}-1H-INDOL-4-YL)OXY]-2-METHYLPROPANOIC ACID (three-letter code: DRD) (formula: C<sub>35</sub>H<sub>35</sub>NO<sub>5</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			41	35	1	5		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	35	Total 35	O 35	0	0
3	B	42	Total 42	O 42	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.76Å 89.78Å 58.77Å 90.00° 90.32° 90.00°	Depositor
Resolution (Å)	30.00 – 2.34 29.39 – 2.33	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.34) 98.4 (29.39-2.33)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.21 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, $R_{free}$	0.233 , 0.316 0.231 , 0.304	Depositor DCC
$R_{free}$ test set	1267 reflections (5.39%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.6	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 42.4	EDS
Estimated twinning fraction	0.004 for l,k,-h 0.029 for h,-k,-l 0.019 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 24925 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	4231	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.21% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.95	1/2131 (0.0%)	0.87	3/2868 (0.1%)
1	B	1.01	0/2049	0.96	4/2759 (0.1%)
All	All	0.98	1/4180 (0.0%)	0.91	7/5627 (0.1%)

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	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	369	GLU	CG-CD	5.09	1.59	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	318	LEU	CB-CG-CD2	-6.41	100.11	111.00
1	B	212	ARG	NE-CZ-NH2	-6.29	117.15	120.30
1	B	318	LEU	CA-CB-CG	5.85	128.75	115.30
1	B	380	ASP	CB-CG-OD1	5.17	122.95	118.30
1	B	212	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	A	397	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	A	476	LEU	CA-CB-CG	5.04	126.90	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	B	357	ARG	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	2096	0	2157	46	0
1	B	2017	0	2069	35	0
2	A	41	0	34	8	0
3	A	35	0	0	5	0
3	B	42	0	0	6	0
All	All	4231	0	4260	83	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 10.

All (83) 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:A:101:DRD:HAP	2:A:101:DRD:HAK2	1.49	0.94
1:B:364:MET:HE3	3:B:6:HOH:O	1.74	0.88
1:B:271:GLN:HG3	1:B:272:GLU:H	1.40	0.84
1:B:378:GLU:HG2	3:B:57:HOH:O	1.79	0.82
1:A:463:MET:HG3	1:A:464:SER:H	1.46	0.80
1:B:342:SER:O	1:B:345:GLN:HG3	1.81	0.80
1:A:477:TYR:O	1:A:477:TYR:HD1	1.67	0.78
1:B:271:GLN:HG3	1:B:272:GLU:N	1.99	0.78
1:A:275:LYS:HG2	1:A:279:ILE:HG21	1.68	0.76
1:B:283:GLN:NE2	1:B:462:ASP:OD2	2.20	0.75
1:A:463:MET:HG3	1:A:464:SER:N	2.03	0.72
1:A:216:LYS:HE2	1:A:216:LYS:O	1.93	0.69
2:A:101:DRD:HAP	2:A:101:DRD:CAK	2.21	0.69
1:A:449:HIS:HA	1:A:452:LEU:HD22	1.74	0.69
1:A:477:TYR:O	1:A:477:TYR:CD1	2.45	0.69
1:A:260:ASP:C	1:A:262:ILE:H	1.97	0.68
1:A:325:ILE:HD11	1:A:392:ILE:HG13	1.77	0.67
1:A:234:ARG:O	1:A:238:THR:HB	1.96	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:GLU:HG2	3:A:70:HOH:O	1.95	0.66
1:B:443:ARG:O	1:B:447:THR:HG23	1.96	0.65
1:A:474:LYS:HE2	1:A:475:ASP:OD2	1.96	0.64
1:B:325:ILE:HD11	1:B:392:ILE:HG13	1.83	0.60
1:A:370:PHE:HB2	1:A:445:ILE:HD11	1.84	0.60
1:A:238:THR:CG2	1:A:240:LYS:HG3	2.33	0.59
1:A:308:ASN:ND2	1:B:291:GLU:HG2	2.17	0.59
1:B:229:THR:HA	3:B:71:HOH:O	2.04	0.57
1:A:345:GLN:HA	1:A:345:GLN:HE21	1.68	0.57
1:A:457:LYS:HG2	1:A:463:MET:SD	2.45	0.56
1:A:379:LEU:HD11	1:A:435:LEU:HD13	1.87	0.56
1:A:444:GLN:CB	3:A:72:HOH:O	2.53	0.56
1:B:436:LEU:O	1:B:439:MET:HB2	2.04	0.56
1:A:260:ASP:C	1:A:262:ILE:N	2.59	0.56
1:A:297:THR:OG1	1:A:318:LEU:HD21	2.06	0.56
1:A:275:LYS:HG2	1:A:279:ILE:CG2	2.34	0.56
1:A:444:GLN:HB3	3:A:72:HOH:O	2.06	0.55
1:A:325:ILE:HG23	1:A:388:ILE:HD12	1.90	0.54
1:B:451:GLN:HA	1:B:454:GLN:HG2	1.89	0.54
1:A:449:HIS:O	1:A:452:LEU:HB2	2.08	0.53
1:A:330:LEU:HD21	2:A:101:DRD:HAB2	1.91	0.53
1:B:392:ILE:HG22	1:B:393:LEU:HD22	1.92	0.52
1:A:367:LYS:HG2	2:A:101:DRD:HAA2	1.92	0.52
1:B:252:MET:SD	1:B:277:VAL:HG11	2.49	0.52
1:B:208:SER:O	1:B:212:ARG:HG2	2.10	0.51
1:B:289:SER:O	1:B:293:VAL:HG23	2.10	0.51
1:A:363:PHE:CZ	1:A:452:LEU:HB3	2.45	0.51
1:A:440:THR:O	1:A:444:GLN:HG3	2.11	0.50
1:B:319:LYS:HE3	1:B:320:TYR:CE1	2.47	0.50
1:B:275:LYS:HE3	1:B:462:ASP:CG	2.32	0.49
1:B:364:MET:CE	3:B:6:HOH:O	2.44	0.49
2:A:101:DRD:CAK	2:A:101:DRD:CAP	2.90	0.48
1:B:257:MET:O	1:B:261:LYS:HB2	2.13	0.47
1:A:433:ALA:O	1:A:437:GLN:HG3	2.15	0.47
1:A:328:THR:HG21	1:A:388:ILE:HD11	1.97	0.46
1:B:463:MET:SD	1:B:465:LEU:HD13	2.56	0.46
1:B:363:PHE:HE1	1:B:449:HIS:CE1	2.34	0.46
1:A:242:THR:HG23	1:A:242:THR:O	2.14	0.45
1:A:341:ILE:HD12	2:A:101:DRD:HAV	1.97	0.45
1:A:238:THR:HG22	1:A:240:LYS:HG3	1.97	0.45
1:B:259:GLU:HA	1:B:259:GLU:OE2	2.16	0.45

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:ASN:HB3	3:A:16:HOH:O	2.15	0.45
1:B:238:THR:HB	1:B:239:GLY:H	1.50	0.44
1:B:363:PHE:CE1	1:B:449:HIS:CE1	3.05	0.44
1:A:288:ARG:HG3	2:A:101:DRD:HBN3	1.99	0.43
1:B:212:ARG:HD2	1:B:212:ARG:HA	1.84	0.43
1:B:438:LYS:HA	1:B:438:LYS:HD2	1.59	0.43
1:B:368:PHE:O	1:B:372:VAL:HG23	2.18	0.43
1:A:307:VAL:HG22	3:A:25:HOH:O	2.18	0.42
1:A:238:THR:HG22	1:A:240:LYS:H	1.84	0.42
1:B:286:GLN:OE1	1:B:465:LEU:HG	2.20	0.42
1:B:241:THR:O	1:B:243:ASP:OD1	2.37	0.42
1:A:288:ARG:NH1	1:A:291:GLU:OE1	2.53	0.41
1:A:477:TYR:C	1:A:477:TYR:CD1	2.93	0.41
1:B:386:ILE:HB	1:B:417:LEU:HD13	2.03	0.41
1:A:437:GLN:O	1:A:440:THR:HG23	2.20	0.41
2:A:101:DRD:HAK2	2:A:101:DRD:CAP	2.35	0.41
1:B:467:PRO:HA	3:B:36:HOH:O	2.20	0.41
1:A:316:THR:O	1:A:320:TYR:HD1	2.03	0.41
1:A:466:HIS:HA	1:A:467:PRO:HD2	1.78	0.41
1:A:325:ILE:HG12	1:A:388:ILE:HG23	2.03	0.40
1:A:360:PHE:CE1	1:A:456:ILE:HD11	2.55	0.40
1:B:447:THR:HG23	3:B:46:HOH:O	2.21	0.40
1:B:421:LEU:HD11	1:B:435:LEU:HD23	2.04	0.40
1:A:301:LYS:HZ2	1:B:467:PRO:N	2.19	0.40

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	257/271 (95%)	239 (93%)	12 (5%)	6 (2%)	<b>8</b> <b>5</b>

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	249/271 (92%)	237 (95%)	10 (4%)	2 (1%)	24	25
All	All	506/542 (93%)	476 (94%)	22 (4%)	8 (2%)	12	9

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	358	LYS
1	A	464	SER
1	B	274	SER
1	A	243	ASP
1	A	261	LYS
1	A	465	LEU
1	B	239	GLY
1	A	467	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	234/244 (96%)	212 (91%)	22 (9%)	11	10
1	B	226/244 (93%)	203 (90%)	23 (10%)	9	8
All	All	460/488 (94%)	415 (90%)	45 (10%)	10	9

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	207	GLU
1	A	216	LYS
1	A	234	ARG
1	A	238	THR
1	A	242	THR
1	A	243	ASP
1	A	248	VAL
1	A	255	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	264	PHE
1	A	302	SER
1	A	318	LEU
1	A	322	VAL
1	A	342	SER
1	A	345	GLN
1	A	404	LYS
1	A	440	THR
1	A	441	ASP
1	A	452	LEU
1	A	453	LEU
1	A	456	ILE
1	A	465	LEU
1	A	477	TYR
1	B	207	GLU
1	B	208	SER
1	B	234	ARG
1	B	240	LYS
1	B	241	THR
1	B	248	VAL
1	B	259	GLU
1	B	260	ASP
1	B	262	ILE
1	B	289	SER
1	B	318	LEU
1	B	322	VAL
1	B	323	HIS
1	B	343	GLU
1	B	363	PHE
1	B	364	MET
1	B	402	ASN
1	B	411	ASP
1	B	428	SER
1	B	440	THR
1	B	441	ASP
1	B	452	LEU
1	B	464	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	294	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	345	GLN
1	B	253	ASN
1	B	271	GLN
1	B	273	GLN
1	B	402	ASN
1	B	437	GLN

### 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 ⓘ

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	$\# Z  > 2$
2	DRD	A	101	-	40,45,45	1.55	7 (17%)	55,64,64	1.38	4 (7%)

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	DRD	A	101	-	-	0/23/29/29	0/5/5/5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	101	DRD	CAO-NAT	-5.18	1.33	1.39
2	A	101	DRD	CAU-NAT	-2.47	1.35	1.38
2	A	101	DRD	CBH-CBC	2.02	1.40	1.37
2	A	101	DRD	CAE-CBK	2.63	1.42	1.38
2	A	101	DRD	OAF-CAG	2.91	1.49	1.45
2	A	101	DRD	CBC-CBB	3.22	1.55	1.49
2	A	101	DRD	CBA-CBB	3.37	1.55	1.49

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	101	DRD	OAD-CAE-CBJ	-2.78	118.21	124.01
2	A	101	DRD	OAF-CAS-CAN	3.00	118.25	114.30
2	A	101	DRD	OAD-CAE-CBK	3.83	120.95	116.11
2	A	101	DRD	CAG-OAF-CAS	4.79	129.13	120.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	101	DRD	8	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	261/271 (96%)	0.35	17 (6%)	22 33	19, 35, 66, 96	0
1	B	253/271 (93%)	0.45	25 (9%)	9 16	15, 31, 83, 119	0
All	All	514/542 (94%)	0.40	42 (8%)	14 22	15, 33, 75, 119	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	465	LEU	11.8
1	A	264	PHE	9.0
1	B	241	THR	7.8
1	B	467	PRO	7.6
1	B	272	GLU	6.7
1	B	464	SER	6.4
1	B	273	GLN	6.2
1	B	274	SER	6.0
1	B	242	THR	5.9
1	B	243	ASP	5.8
1	A	477	TYR	5.5
1	A	262	ILE	5.2
1	B	240	LYS	4.6
1	B	466	HIS	4.6
1	A	242	THR	4.6
1	B	454	GLN	4.2
1	B	260	ASP	4.1
1	B	461	THR	4.1
1	B	463	MET	4.0
1	B	244	LYS	3.8
1	A	287	PHE	3.8
1	B	363	PHE	3.7
1	A	275	LYS	3.3
1	B	439	MET	3.3

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	239	GLY	3.1
1	A	241	THR	3.0
1	B	262	ILE	2.9
1	B	259	GLU	2.9
1	A	243	ASP	2.7
1	B	257	MET	2.7
1	A	463	MET	2.7
1	B	457	LYS	2.4
1	A	263	LYS	2.3
1	A	452	LEU	2.3
1	A	277	VAL	2.3
1	A	436	LEU	2.3
1	A	470	GLN	2.3
1	A	244	LYS	2.2
1	B	286	GLN	2.2
1	A	311	LEU	2.1
1	A	260	ASP	2.1
1	B	462	ASP	2.0

## 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
2	DRD	A	101	41/41	0.71	0.26	2.75	60,75,76,77	0

## 6.5 Other polymers

There are no such residues in this entry.