



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:40 PM GMT

PDB ID : 4A4V  
Title : Ligand binding domain of human PPAR gamma in complex with amorfrutin 2  
Authors : de Groot, J.C.; Weidner, C.; Krausze, J.; Kawamoto, K.; Schroeder, F.C.; Sauer, S.; Buessow, K.  
Deposited on : 2011-10-20  
Resolution : 2.00 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.

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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

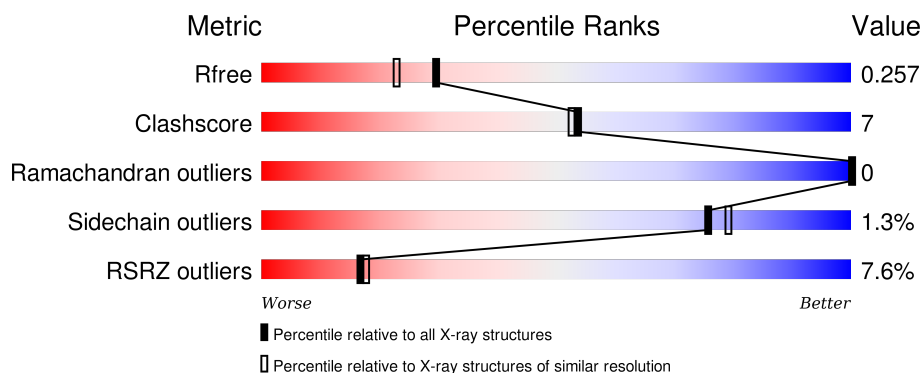
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (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  $\geq 3$ , 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	287	<div> <div>5%</div> <div>79% 13% 8%</div> </div>
1	B	287	<div> <div>9%</div> <div>78% 14% 8%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4671 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.

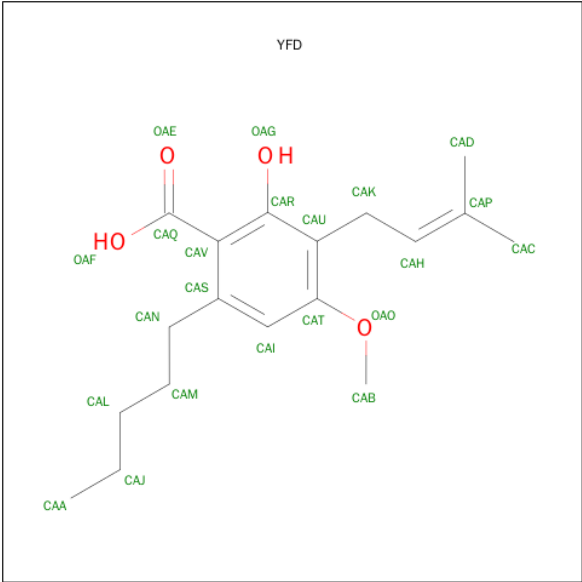
- Molecule 1 is a protein called PEROXISOME PROLIFERATOR-ACTIVATED RECEPTOR GAMMA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	14	0
			2193	1418	354	410	11			
1	B	265	Total	C	N	O	S	0	11	0
			2187	1422	353	399	13			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	191	GLY	-	EXPRESSION TAG	UNP P37231
A	192	SER	-	EXPRESSION TAG	UNP P37231
A	193	HIS	-	EXPRESSION TAG	UNP P37231
A	194	MET	-	EXPRESSION TAG	UNP P37231
B	191	GLY	-	EXPRESSION TAG	UNP P37231
B	192	SER	-	EXPRESSION TAG	UNP P37231
B	193	HIS	-	EXPRESSION TAG	UNP P37231
B	194	MET	-	EXPRESSION TAG	UNP P37231

- Molecule 2 is AMORFRUTIN 2 (three-letter code: YFD) (formula: C<sub>18</sub>H<sub>26</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			22	18	4		
2	B	1	Total	C	O	0	0
			22	18	4		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	135	Total	O	0	0
			135	135		
3	B	112	Total	O	0	0
			112	112		



- Molecule 1: PEROXISOME PROLIFERATOR-ACTIVATED RECEPTOR GAMMA



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.29 Å   60.97 Å   117.90 Å 90.00°   102.65°   90.00°	Depositor
Resolution (Å)	27.45 – 2.00 27.08 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (27.45-2.00) 99.1 (27.08-2.00)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.69 (at 1.99 Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.209   ,   0.259 0.208   ,   0.257	Depositor DCC
$R_{free}$ test set	2151 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.0	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 47.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 43007 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4671	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.67% 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: YFD

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	0.51	0/2264	0.60	0/3046
1	B	0.49	0/2255	0.57	0/3032
All	All	0.50	0/4519	0.59	0/6078

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	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	A	240	LYS	Peptide
1	A	241	THR	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	2193	0	2285	27	0
1	B	2187	0	2291	33	0
2	A	22	0	24	1	0
2	B	22	0	25	6	0
3	A	135	0	0	0	0
3	B	112	0	0	1	0
All	All	4671	0	4625	59	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 7.

All (59) 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:275:LYS:HD2	1:B:276:GLU:H	1.04	1.18
1:B:275:LYS:HD2	1:B:276:GLU:N	1.86	0.90
1:B:275:LYS:CD	1:B:276:GLU:H	1.90	0.83
1:A:205:ASN:HB2	1:A:206:PRO:HD2	1.60	0.81
1:A:440:THR:HG21	1:B:443:ARG:HD2	1.73	0.70
1:A:325:ILE:HD11	1:A:392:ILE:HG13	1.75	0.68
1:A:439[A]:MET:HE1	1:B:437:GLN:HG2	1.77	0.67
1:A:359:PRO:HG2	1:A:456:ILE:HD13	1.78	0.65
1:A:360:PHE:O	1:A:363:PHE:HD1	1.79	0.65
1:B:290:VAL:HG21	1:B:473:TYR:HD1	1.62	0.63
1:B:451:GLN:O	1:B:454[A]:GLN:HG2	2.00	0.62
1:B:290:VAL:HG21	1:B:473:TYR:CD1	2.37	0.59
1:A:241:THR:HG23	1:A:244[B]:LYS:H	1.68	0.58
1:A:241:THR:HG23	1:A:244[A]:LYS:H	1.68	0.58
2:B:999:YFD:OAG	2:B:999:YFD:OAF	2.21	0.57
1:A:252:MET:O	1:A:256:MET:HG2	2.04	0.56
1:B:325:ILE:HD11	1:B:392:ILE:HG13	1.88	0.55
1:A:205:ASN:HB2	1:A:206:PRO:CD	2.32	0.55
1:A:325:ILE:HD11	1:A:392:ILE:CG1	2.36	0.54
1:B:430:GLN:O	1:B:434:LYS:HG3	2.08	0.53
1:B:325:ILE:HD11	1:B:392:ILE:CG1	2.39	0.52
1:A:459:THR:HG23	1:A:460:GLU:HG2	1.92	0.51
1:A:439[A]:MET:CE	1:B:437:GLN:HG2	2.42	0.49
1:A:370:PHE:CB	1:A:445:ILE:HD11	2.43	0.48
1:A:323:HIS:CE1	1:A:473:TYR:CE1	3.01	0.47
1:B:439[B]:MET:HE3	1:B:439[B]:MET:HA	1.97	0.47
1:A:285:CYS:SG	2:A:999:YFD:HAD2	2.53	0.47
1:A:394:SER:O	1:A:397:ARG:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:PHE:HB2	1:A:445:ILE:HD11	1.96	0.47
1:B:330:LEU:HD22	2:B:999:YFD:HAB2	1.97	0.46
1:B:439[B]:MET:CE	1:B:439[B]:MET:HA	2.45	0.46
1:B:297:THR:O	1:B:301:LYS:HG2	2.14	0.46
1:A:452:LEU:O	1:A:456:ILE:HG12	2.16	0.45
1:B:285[B]:CYS:SG	2:B:999:YFD:HAD3	2.57	0.44
1:B:234:ARG:HD2	3:B:2032:HOH:O	2.17	0.44
1:A:258:GLY:O	1:A:261[B]:LYS:HG3	2.16	0.44
1:A:219:TYR:CZ	1:A:223:ILE:HD11	2.53	0.43
1:A:322:VAL:HG21	1:A:472:ILE:HD13	1.99	0.43
1:B:292:ALA:HB1	2:B:999:YFD:HAA2	2.00	0.43
2:B:999:YFD:HA1	2:B:999:YFD:HAB3	1.70	0.43
1:B:466:HIS:HA	1:B:467:PRO:HD3	1.88	0.43
1:B:360:PHE:O	1:B:363[B]:PHE:HD1	2.01	0.43
1:B:402:ASN:O	1:B:405:PRO:HD2	2.19	0.43
1:A:433:ALA:O	1:A:437:GLN:HG3	2.19	0.43
1:B:448:GLU:O	1:B:451:GLN:HG3	2.19	0.42
1:B:365:GLU:HB3	1:B:366:PRO:HD3	2.01	0.42
1:A:455:VAL:O	1:A:459:THR:HG22	2.19	0.42
1:B:320:TYR:CZ	1:B:398:PRO:HG2	2.55	0.42
1:B:212:ARG:HA	1:B:212:ARG:HD2	1.85	0.42
1:B:275:LYS:CD	1:B:276:GLU:N	2.66	0.41
1:B:466:HIS:HB3	1:B:469:LEU:HD12	2.02	0.41
1:B:282:PHE:HE1	1:B:363[A]:PHE:CE1	2.38	0.41
1:B:214:LEU:HD23	1:B:416:ALA:HB2	2.02	0.41
1:B:285[B]:CYS:SG	2:B:999:YFD:CAP	3.09	0.41
1:B:276:GLU:CD	1:B:357:ARG:HE	2.24	0.41
1:B:462:ASP:HB3	1:B:465:LEU:H	1.86	0.40
1:A:219:TYR:CE1	1:A:223:ILE:HD11	2.57	0.40

There are no symmetry-related clashes.

## 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	274/287 (96%)	268 (98%)	6 (2%)	0	100	100
1	B	272/287 (95%)	264 (97%)	8 (3%)	0	100	100
All	All	546/574 (95%)	532 (97%)	14 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	251/258 (97%)	248 (99%)	3 (1%)	78	81
1	B	249/258 (96%)	245 (98%)	4 (2%)	70	73
All	All	500/516 (97%)	493 (99%)	7 (1%)	76	77

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	402[A]	ASN
1	A	402[B]	ASN
1	A	470	GLN
1	B	241	THR
1	B	270	LEU
1	B	275	LYS
1	B	457	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	410	GLN
1	B	308	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 ⓘ

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	YFD	A	999	-	19,22,22	1.68	3 (15%)	24,29,29	2.13	6 (25%)
2	YFD	B	999	-	19,22,22	1.52	2 (10%)	24,29,29	2.46	7 (29%)

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	YFD	A	999	-	-	0/12/16/16	0/1/1/1
2	YFD	B	999	-	-	0/12/16/16	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	999	YFD	CAK-CAH	-4.73	1.41	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	999	YFD	CAK-CAH	-4.69	1.41	1.50
2	B	999	YFD	CAH-CAP	2.64	1.40	1.32
2	A	999	YFD	CAH-CAP	2.98	1.41	1.32
2	A	999	YFD	CAK-CAU	3.29	1.55	1.51

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	999	YFD	CAB-OAO-CAT	-5.08	109.84	117.54
2	B	999	YFD	OAO-CAT-CAI	-4.83	115.97	124.21
2	B	999	YFD	CAB-OAO-CAT	-4.46	110.78	117.54
2	A	999	YFD	OAO-CAT-CAI	-3.85	117.64	124.21
2	A	999	YFD	CAN-CAS-CAI	-2.33	114.43	119.31
2	B	999	YFD	CAN-CAS-CAI	-2.24	114.62	119.31
2	B	999	YFD	CAC-CAP-CAD	2.19	120.01	114.64
2	B	999	YFD	CAR-CAV-CAS	2.20	120.78	118.66
2	B	999	YFD	CAN-CAS-CAV	2.65	127.13	122.52
2	A	999	YFD	CAK-CAH-CAP	3.15	131.50	127.61
2	A	999	YFD	CAN-CAS-CAV	3.30	128.25	122.52
2	A	999	YFD	OAO-CAT-CAU	5.32	120.65	115.43
2	B	999	YFD	OAO-CAT-CAU	7.67	122.95	115.43

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	999	YFD	1	0
2	B	999	YFD	6	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	264/287 (91%)	0.15	14 (5%)	30 32	20, 36, 68, 84	0
1	B	265/287 (92%)	0.44	26 (9%)	10 10	21, 39, 83, 102	0
All	All	529/574 (92%)	0.30	40 (7%)	17 18	20, 37, 78, 102	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	241	THR	8.7
1	B	463	MET	8.6
1	B	464	SER	6.4
1	A	204	LEU	5.5
1	B	269	PRO	5.4
1	A	203	GLN	5.2
1	B	243	ASP	5.1
1	B	206	PRO	4.9
1	B	465	LEU	4.8
1	B	207	GLU	4.7
1	A	477	TYR	4.3
1	B	263	LYS	4.1
1	B	244	LYS	4.1
1	B	240	LYS	4.0
1	B	270	LEU	3.9
1	B	242	THR	3.8
1	A	262	ILE	3.8
1	B	239	GLY	3.4
1	B	462	ASP	3.3
1	A	274	SER	3.2
1	A	260	ASP	3.0
1	B	451	GLN	2.8
1	A	476	LEU	2.8
1	A	240	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	261[A]	LYS	2.8
1	B	341	ILE	2.7
1	A	475	ASP	2.6
1	B	262	ILE	2.6
1	B	238	THR	2.5
1	B	362[A]	ASP	2.4
1	A	275[A]	LYS	2.4
1	B	340	LEU	2.2
1	B	458	LYS	2.2
1	B	454[A]	GLN	2.2
1	A	472	ILE	2.2
1	B	339	VAL	2.1
1	A	206	PRO	2.1
1	A	241	THR	2.0
1	B	260	ASP	2.1
1	B	256	MET	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( $\text{\AA}^2$ )	Q<0.9
2	YFD	A	999	22/22	0.80	0.18	0.48	42,47,49,52	0
2	YFD	B	999	22/22	0.89	0.14	-0.42	18,32,38,40	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.