



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:06 AM GMT

PDB ID : 2ZK0  
Title : Human peroxisome proliferator-activated receptor gamma ligand binding domain  
Authors : Waku, T.; Shiraki, T.; Oyama, T.; Fujimoto, Y.; Morikawa, K.  
Deposited on : 2008-03-12  
Resolution : 2.36 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

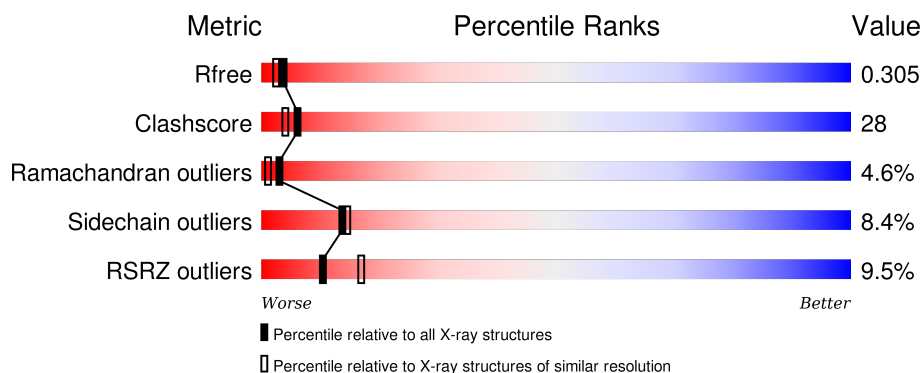
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.36 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	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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	286	<div> <div>9%</div> <div>53% 35% 6% • 6%</div> </div>
1	B	286	<div> <div>8%</div> <div>52% 32% 6% • 9%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4303 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	270	Total	C	N	O	S	0	0	0
			2166	1397	354	405	10			
1	B	259	Total	C	N	O	S	0	0	0
			2078	1343	341	385	9			

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 water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	26	Total	O	0	0
			26	26		
2	B	33	Total	O	0	0
			33	33		

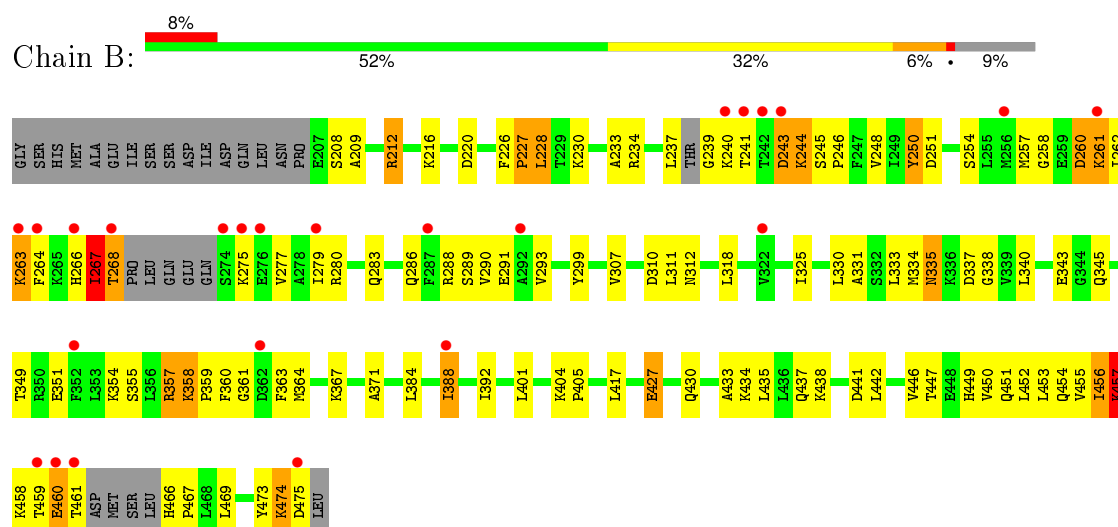
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 gamma



- 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, $\alpha$ , $\beta$ , $\gamma$	92.75Å 61.66Å 118.60Å 90.00° 102.69° 90.00°	Depositor
Resolution (Å)	32.77 – 2.36 48.92 – 2.34	Depositor EDS
% Data completeness (in resolution range)	92.9 (32.77-2.36) 91.9 (48.92-2.34)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.24 (at 2.34Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.249 , 0.313 0.247 , 0.305	Depositor DCC
$R_{free}$ test set	1213 reflections (4.81%)	DCC
Wilson B-factor (Å <sup>2</sup> )	42.9	Xtriage
Anisotropy	0.541	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 41.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 26963 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	4303	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.38% 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

### 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	0.47	0/2203	0.71	3/2967 (0.1%)
1	B	0.46	0/2111	0.67	0/2838
All	All	0.46	0/4314	0.69	3/5805 (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

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	475	ASP	N-CA-C	8.06	132.76	111.00
1	A	275	LYS	N-CA-C	-7.96	89.50	111.00
1	A	473	TYR	N-CA-C	6.75	129.22	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	250	TYR	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	2166	0	2232	130	0
1	B	2078	0	2142	113	0
2	A	26	0	0	2	0
2	B	33	0	0	1	0
All	All	4303	0	4374	243	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 28.

All (243) 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:A:267:ILE:HG22	1:A:280:ARG:HG3	1.31	1.11
1:B:357:ARG:HD3	1:B:359:PRO:HD2	1.34	1.07
1:A:235:ALA:HA	1:A:240:LYS:HD3	1.37	1.06
1:A:273:GLN:O	1:A:276:GLU:HA	1.59	1.03
1:B:212:ARG:HB3	1:B:212:ARG:HH11	1.16	1.02
1:B:258:GLY:O	1:B:262:ILE:HG22	1.62	0.98
1:A:286:GLN:HE22	1:A:465:LEU:HA	1.34	0.92
1:B:357:ARG:CD	1:B:359:PRO:HD2	1.99	0.92
1:B:335:ASN:ND2	1:B:337:ASP:H	1.72	0.88
1:B:335:ASN:HD22	1:B:335:ASN:C	1.80	0.85
1:A:325:ILE:HG23	1:A:388:ILE:HD12	1.56	0.85
1:A:270:LEU:HB3	1:A:275:LYS:CB	2.05	0.85
1:B:457:LYS:NZ	1:B:461:THR:HA	1.91	0.84
1:A:267:ILE:CG2	1:A:280:ARG:HG3	2.09	0.82
1:B:384:LEU:O	1:B:388:ILE:HG23	1.79	0.81
1:A:325:ILE:HD13	1:A:388:ILE:HG23	1.62	0.81
1:A:269:PRO:HG3	2:A:1049:HOH:O	1.81	0.79
1:A:476:LEU:HD23	1:A:476:LEU:OXT	1.82	0.79
1:B:447:THR:O	1:B:451:GLN:HG2	1.82	0.79
1:A:270:LEU:O	1:A:275:LYS:HB3	1.83	0.78
1:B:279:ILE:O	1:B:283:GLN:HG3	1.83	0.78
1:A:349:THR:HG22	1:A:351:GLU:H	1.49	0.78
1:A:271:GLN:OE1	1:A:271:GLN:N	2.17	0.77
1:B:434:LYS:HA	1:B:437:GLN:HE21	1.50	0.77
1:A:357:ARG:HG2	1:A:359:PRO:HD2	1.67	0.77
1:A:267:ILE:HG13	1:A:283:GLN:HB2	1.68	0.76
1:A:272:GLU:C	1:A:274:SER:H	1.89	0.76
1:A:274:SER:C	1:A:276:GLU:N	2.37	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:GLN:O	1:A:276:GLU:HG2	1.87	0.75
1:B:456:ILE:O	1:B:458:LYS:N	2.21	0.74
1:A:274:SER:O	1:A:276:GLU:N	2.20	0.73
1:B:266:HIS:O	1:B:267:ILE:HG23	1.90	0.71
1:B:257:MET:HG3	1:B:261:LYS:HD3	1.70	0.71
1:B:357:ARG:HD3	1:B:359:PRO:CD	2.17	0.71
1:A:293:VAL:HG22	1:A:322:VAL:HG11	1.73	0.70
1:B:212:ARG:CB	1:B:212:ARG:HH11	1.99	0.70
1:A:368:PHE:O	1:A:372:VAL:HG23	1.91	0.70
1:A:305:GLY:HA2	1:A:308:ASN:HD22	1.57	0.69
1:A:441:ASP:O	1:A:445:ILE:HG12	1.93	0.69
1:A:266:HIS:CD2	1:A:287:PHE:HB2	2.29	0.68
1:A:272:GLU:HG3	1:A:274:SER:HB2	1.76	0.67
1:B:457:LYS:HZ2	1:B:461:THR:HA	1.57	0.67
1:A:271:GLN:O	1:A:272:GLU:O	2.14	0.66
1:B:457:LYS:HZ3	1:B:461:THR:HA	1.59	0.66
1:A:270:LEU:HB3	1:A:275:LYS:HB3	1.77	0.66
1:B:251:ASP:HB2	1:B:254:SER:OG	1.97	0.65
1:A:273:GLN:HG2	1:A:273:GLN:O	1.96	0.64
1:B:335:ASN:ND2	1:B:338:GLY:H	1.95	0.63
1:A:272:GLU:O	1:A:274:SER:N	2.31	0.63
1:A:473:TYR:C	1:A:475:ASP:H	2.00	0.63
1:B:456:ILE:C	1:B:458:LYS:H	2.01	0.63
1:A:274:SER:C	1:A:276:GLU:H	2.00	0.63
1:A:212:ARG:HD3	1:A:419:LEU:HD13	1.80	0.63
1:B:241:THR:HG22	1:B:241:THR:O	1.98	0.63
1:A:325:ILE:HD11	1:A:392:ILE:HG13	1.81	0.63
1:B:248:VAL:HG12	1:B:250:TYR:HD2	1.64	0.62
1:B:263:LYS:NZ	1:B:263:LYS:HB3	2.13	0.62
1:B:457:LYS:HA	1:B:457:LYS:NZ	2.15	0.62
1:A:259:GLU:HG2	1:A:269:PRO:HD2	1.82	0.61
1:B:288:ARG:HD2	1:B:288:ARG:O	2.00	0.61
1:A:270:LEU:HB3	1:A:275:LYS:CG	2.30	0.61
1:B:262:ILE:CG2	1:B:264:PHE:HE1	2.14	0.61
1:B:456:ILE:O	1:B:459:THR:N	2.33	0.61
1:B:290:VAL:HG21	1:B:473:TYR:CD1	2.36	0.61
1:A:207:GLU:HG3	1:A:209:ALA:H	1.65	0.60
1:B:335:ASN:HD22	1:B:337:ASP:H	1.44	0.59
1:A:268:THR:OG1	1:A:269:PRO:HD2	2.01	0.59
1:B:330:LEU:HD22	1:B:334:MET:CE	2.31	0.59
1:A:293:VAL:HG22	1:A:322:VAL:CG1	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:LEU:O	1:A:472:ILE:HG22	2.01	0.59
1:B:457:LYS:HZ3	1:B:457:LYS:HA	1.66	0.58
1:A:433:ALA:O	1:A:437:GLN:HG3	2.03	0.58
1:A:270:LEU:O	1:A:271:GLN:HG2	2.03	0.58
1:B:325:ILE:HD13	1:B:388:ILE:CD1	2.34	0.58
1:B:325:ILE:HD13	1:B:388:ILE:HD13	1.86	0.57
1:B:334:MET:HE3	1:B:371:ALA:HB2	1.86	0.57
1:B:335:ASN:C	1:B:335:ASN:ND2	2.54	0.57
1:A:379:LEU:HD11	1:A:435:LEU:HD13	1.87	0.57
1:A:264:PHE:C	1:A:266:HIS:H	2.08	0.57
1:B:212:ARG:NH1	1:B:212:ARG:HB3	2.02	0.56
1:A:394:SER:O	1:A:397:ARG:HG2	2.05	0.56
1:A:444:GLN:O	1:A:448:GLU:HB2	2.05	0.56
1:B:264:PHE:HD2	1:B:266:HIS:CE1	2.23	0.56
1:B:335:ASN:ND2	1:B:337:ASP:N	2.49	0.56
1:B:333:LEU:HB3	1:B:340:LEU:HB2	1.87	0.56
1:A:277:VAL:O	1:A:281:ILE:HG13	2.06	0.55
1:A:465:LEU:N	1:A:465:LEU:HD22	2.21	0.55
1:A:449:HIS:CE1	1:A:453:LEU:HD13	2.42	0.55
1:B:466:HIS:HB3	1:B:467:PRO:HD3	1.87	0.55
1:A:273:GLN:HE21	1:A:273:GLN:H	1.53	0.55
1:A:276:GLU:CD	1:A:357:ARG:HH21	2.09	0.55
1:A:207:GLU:OE1	1:A:207:GLU:HA	2.07	0.55
1:A:268:THR:O	1:A:269:PRO:O	2.25	0.54
1:A:270:LEU:CB	1:A:275:LYS:HG2	2.37	0.54
1:A:448:GLU:O	1:A:452:LEU:HG	2.08	0.54
1:B:216:LYS:NZ	1:B:220:ASP:OD1	2.39	0.54
1:B:262:ILE:HG12	1:B:263:LYS:H	1.72	0.54
1:A:267:ILE:HG21	1:A:280:ARG:HA	1.90	0.54
1:A:255:LEU:HD22	1:A:277:VAL:HG23	1.89	0.54
1:B:359:PRO:HG2	1:B:360:PHE:CD2	2.42	0.53
1:A:208:SER:HB2	1:A:419:LEU:HD11	1.90	0.53
1:A:403:VAL:O	1:A:407:GLU:HG3	2.09	0.53
1:A:365:GLU:OE1	1:A:365:GLU:HA	2.08	0.53
1:B:456:ILE:C	1:B:458:LYS:N	2.62	0.53
1:A:265:LYS:HG2	1:A:265:LYS:O	2.08	0.53
1:A:277:VAL:HG13	1:A:278:ALA:N	2.25	0.52
1:A:469:LEU:O	1:A:473:TYR:HD2	1.93	0.52
1:B:442:LEU:O	1:B:446:VAL:HG23	2.09	0.52
1:A:286:GLN:HE22	1:A:465:LEU:CA	2.15	0.52
1:A:272:GLU:CG	1:A:274:SER:HB2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:TYR:C	1:A:475:ASP:N	2.63	0.51
1:B:277:VAL:HA	1:B:280:ARG:NH1	2.24	0.51
1:A:276:GLU:CG	1:A:357:ARG:HH21	2.23	0.51
1:B:299:TYR:CD2	1:B:388:ILE:HD11	2.45	0.51
1:B:335:ASN:HD21	1:B:338:GLY:N	2.08	0.51
1:B:251:ASP:H	1:B:254:SER:HB2	1.74	0.51
1:B:330:LEU:HD22	1:B:334:MET:HE1	1.93	0.51
1:A:443:ARG:HH11	1:A:443:ARG:HG3	1.75	0.51
1:B:263:LYS:C	1:B:263:LYS:HD2	2.31	0.50
1:A:443:ARG:NH1	1:A:443:ARG:HG3	2.26	0.50
1:B:228:LEU:HD13	1:B:333:LEU:HD22	1.93	0.50
1:A:267:ILE:HG22	1:A:280:ARG:CG	2.21	0.50
1:B:307:VAL:HG22	2:B:1041:HOH:O	2.11	0.50
1:B:262:ILE:HD11	1:B:345:GLN:CB	2.42	0.50
1:A:393:LEU:HD12	1:A:409:ILE:HB	1.93	0.50
1:A:311:LEU:C	1:A:311:LEU:HD13	2.31	0.50
1:B:358:LYS:HB3	1:B:359:PRO:CD	2.42	0.49
1:A:466:HIS:CE1	1:A:468:LEU:HB2	2.46	0.49
1:B:460:GLU:OE1	1:B:461:THR:N	2.45	0.49
1:A:255:LEU:CD2	1:A:277:VAL:HG23	2.42	0.49
1:A:270:LEU:C	1:A:271:GLN:OE1	2.50	0.49
1:B:262:ILE:HD11	1:B:345:GLN:HB2	1.94	0.49
1:A:350:ARG:HG3	1:A:368:PHE:CD2	2.48	0.49
1:B:438:LYS:HA	1:B:441:ASP:OD1	2.12	0.49
1:B:263:LYS:HB3	1:B:263:LYS:HZ2	1.77	0.48
1:A:348:MET:SD	1:A:353:LEU:HD21	2.53	0.48
1:A:383:ASP:OD2	1:A:425:HIS:HE1	1.96	0.48
1:B:289:SER:O	1:B:293:VAL:HG23	2.13	0.48
1:A:266:HIS:CD2	1:A:287:PHE:CB	2.97	0.48
1:A:212:ARG:HH12	1:A:420:GLN:HA	1.78	0.48
1:B:330:LEU:O	1:B:334:MET:HG3	2.14	0.48
1:A:325:ILE:HD11	1:A:392:ILE:CG1	2.44	0.48
1:B:473:TYR:O	1:B:474:LYS:O	2.33	0.47
1:A:363:PHE:CE1	1:A:452:LEU:HB2	2.50	0.47
1:A:357:ARG:NH1	1:A:460:GLU:CD	2.68	0.47
1:A:291:GLU:HA	1:A:294:GLN:NE2	2.29	0.47
1:A:401:LEU:C	1:A:402:ASN:HD22	2.18	0.47
1:A:272:GLU:C	1:A:274:SER:N	2.54	0.47
1:B:288:ARG:HH11	1:B:291:GLU:HB2	1.80	0.47
1:A:270:LEU:O	1:A:275:LYS:CB	2.59	0.47
1:A:266:HIS:CE1	1:A:291:GLU:OE2	2.67	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:404:LYS:HB3	1:B:405:PRO:CD	2.45	0.47
1:A:270:LEU:HB3	1:A:275:LYS:HG2	1.96	0.47
1:B:325:ILE:HD11	1:B:392:ILE:CG1	2.44	0.47
1:B:335:ASN:ND2	1:B:338:GLY:N	2.60	0.46
1:B:457:LYS:HA	1:B:460:GLU:O	2.15	0.46
1:B:234:ARG:O	1:B:239:GLY:HA3	2.15	0.46
1:B:367:LYS:NZ	1:B:449:HIS:HD2	2.13	0.46
1:B:343:GLU:OE2	1:B:343:GLU:N	2.48	0.46
1:A:288:ARG:HH11	1:A:291:GLU:HB2	1.79	0.46
1:B:417:LEU:HD21	1:B:435:LEU:HD23	1.97	0.46
1:B:357:ARG:HH11	1:B:357:ARG:CG	2.28	0.46
1:A:290:VAL:O	1:A:294:GLN:HG3	2.16	0.46
1:B:277:VAL:HA	1:B:280:ARG:HH12	1.81	0.46
1:B:266:HIS:C	1:B:267:ILE:HG12	2.36	0.46
1:B:457:LYS:HG3	1:B:461:THR:HG23	1.98	0.46
1:A:322:VAL:HG12	1:A:323:HIS:N	2.30	0.46
1:B:262:ILE:CG2	1:B:264:PHE:CE1	2.98	0.46
1:B:267:ILE:HB	1:B:268:THR:H	1.25	0.46
1:A:290:VAL:HG21	1:A:466:HIS:CD2	2.51	0.46
1:B:358:LYS:CB	1:B:359:PRO:CD	2.93	0.46
1:B:257:MET:O	1:B:260:ASP:HB3	2.15	0.46
1:B:430:GLN:HG3	1:B:433:ALA:HB3	1.98	0.46
1:B:262:ILE:HG23	1:B:264:PHE:CE1	2.52	0.45
1:B:331:ALA:HA	1:B:334:MET:HE2	1.97	0.45
1:A:272:GLU:HG3	1:A:274:SER:H	1.81	0.45
1:B:358:LYS:HG2	1:B:359:PRO:N	2.29	0.45
1:B:335:ASN:HD22	1:B:337:ASP:N	2.13	0.45
1:B:330:LEU:HD22	1:B:334:MET:SD	2.56	0.45
1:A:310:ASP:OD2	1:A:312:ASN:HB2	2.16	0.45
1:A:276:GLU:HG3	1:A:357:ARG:HH21	1.82	0.45
1:A:271:GLN:C	1:A:272:GLU:O	2.54	0.45
1:A:273:GLN:O	1:A:276:GLU:CA	2.48	0.45
1:A:262:ILE:HG22	1:A:264:PHE:CD1	2.51	0.45
1:A:472:ILE:O	1:A:472:ILE:HG12	2.16	0.45
1:A:357:ARG:O	1:A:359:PRO:N	2.50	0.44
1:A:259:GLU:HA	1:A:264:PHE:CZ	2.52	0.44
1:A:469:LEU:O	1:A:473:TYR:CD2	2.71	0.44
1:B:452:LEU:O	1:B:456:ILE:HG13	2.18	0.44
1:B:358:LYS:HB3	1:B:359:PRO:HD3	1.99	0.44
1:B:250:TYR:HB3	1:B:349:THR:HG21	2.00	0.44
1:B:310:ASP:OD1	1:B:312:ASN:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:364:MET:O	1:B:367:LYS:HB2	2.18	0.44
1:A:325:ILE:HG23	1:A:388:ILE:CD1	2.40	0.44
1:A:267:ILE:HG13	1:A:283:GLN:CB	2.45	0.43
1:A:388:ILE:HD13	1:A:388:ILE:HA	1.85	0.43
1:B:325:ILE:HD11	1:B:392:ILE:HG13	2.00	0.43
1:A:435:LEU:O	1:A:438:LYS:HB2	2.18	0.43
1:B:286:GLN:O	1:B:289:SER:HB2	2.18	0.43
1:B:237:LEU:C	1:B:239:GLY:N	2.71	0.43
1:B:208:SER:OG	1:B:209:ALA:N	2.51	0.43
1:A:291:GLU:HA	1:A:294:GLN:HE21	1.83	0.43
1:B:243:ASP:O	1:B:244:LYS:HB3	2.18	0.43
1:B:262:ILE:HG12	1:B:263:LYS:N	2.34	0.43
1:B:208:SER:O	1:B:209:ALA:C	2.57	0.43
1:A:219:TYR:CZ	1:A:223:ILE:HD11	2.54	0.43
1:B:243:ASP:CG	1:B:244:LYS:HZ1	2.20	0.43
1:A:387:PHE:CE2	1:A:391:ILE:HD11	2.54	0.42
1:B:427:GLU:N	1:B:427:GLU:OE1	2.52	0.42
1:A:395:GLY:O	1:A:400:LEU:HD12	2.19	0.42
1:A:446:VAL:O	1:A:450:VAL:HG23	2.19	0.42
1:A:230:LYS:O	1:A:234:ARG:HG2	2.18	0.42
1:A:454:GLN:NE2	1:A:454:GLN:HA	2.35	0.42
1:A:270:LEU:C	1:A:271:GLN:CG	2.87	0.42
1:B:267:ILE:C	1:B:268:THR:HG22	2.40	0.42
1:A:472:ILE:O	1:A:475:ASP:OD2	2.38	0.42
1:A:388:ILE:HD13	1:A:391:ILE:HD12	2.01	0.42
1:A:212:ARG:CD	1:A:419:LEU:HD13	2.49	0.42
1:A:272:GLU:HG3	1:A:274:SER:CB	2.48	0.42
1:A:452:LEU:O	1:A:456:ILE:HG12	2.20	0.42
1:B:245:SER:HA	1:B:246:PRO:HD3	1.86	0.42
1:B:310:ASP:OD1	1:B:312:ASN:HB2	2.20	0.42
1:A:261:LYS:HD2	1:A:261:LYS:H	1.85	0.42
1:B:451:GLN:O	1:B:454:GLN:HB3	2.19	0.42
1:B:451:GLN:OE1	1:B:451:GLN:HA	2.21	0.41
1:A:283:GLN:O	1:A:286:GLN:HB2	2.20	0.41
1:A:273:GLN:NE2	1:A:273:GLN:H	2.17	0.41
1:B:447:THR:O	1:B:450:VAL:HG22	2.21	0.41
1:B:226:PHE:HA	1:B:227:PRO:HD3	1.90	0.41
1:A:469:LEU:O	1:A:472:ILE:HG23	2.21	0.41
1:A:475:ASP:HB3	1:A:476:LEU:H	1.21	0.41
1:B:230:LYS:O	1:B:234:ARG:HG2	2.19	0.41
1:A:335:ASN:O	1:A:337:ASP:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:PHE:O	1:A:266:HIS:N	2.52	0.41
1:B:367:LYS:HZ3	1:B:449:HIS:HD2	1.69	0.40
1:B:354:LYS:HA	1:B:361:GLY:O	2.21	0.40
1:A:276:GLU:O	1:A:277:VAL:C	2.59	0.40
1:B:299:TYR:HD2	1:B:388:ILE:HD11	1.86	0.40
1:A:305:GLY:CA	1:A:308:ASN:HD22	2.30	0.40
1:A:425:HIS:HB2	2:A:1046:HOH:O	2.21	0.40
1:B:228:LEU:HD22	1:B:233:ALA:HB2	2.03	0.40
1:A:373:LYS:O	1:A:376:ALA:HB3	2.21	0.40
1:B:266:HIS:ND1	1:B:266:HIS:O	2.54	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	268/286 (94%)	246 (92%)	10 (4%)	12 (4%)	3	1
1	B	251/286 (88%)	226 (90%)	13 (5%)	12 (5%)	3	1
All	All	519/572 (91%)	472 (91%)	23 (4%)	24 (5%)	3	1

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	269	PRO
1	A	272	GLU
1	B	243	ASP
1	B	244	LYS
1	B	267	ILE
1	B	358	LYS
1	B	457	LYS
1	B	474	LYS

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Mol	Chain	Res	Type
1	A	273	GLN
1	A	336	LYS
1	A	475	ASP
1	B	240	LYS
1	B	260	ASP
1	A	260	ASP
1	A	266	HIS
1	A	276	GLU
1	A	457	LYS
1	A	261	LYS
1	A	358	LYS
1	B	275	LYS
1	B	227	PRO
1	B	455	VAL
1	B	456	ILE
1	A	359	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	243/257 (95%)	224 (92%)	19 (8%)	16	17
1	B	232/257 (90%)	211 (91%)	21 (9%)	12	11
All	All	475/514 (92%)	435 (92%)	40 (8%)	14	14

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	216	LYS
1	A	253	ASN
1	A	257	MET
1	A	261	LYS
1	A	263	LYS
1	A	264	PHE
1	A	270	LEU

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Mol	Chain	Res	Type
1	A	271	GLN
1	A	273	GLN
1	A	365	GLU
1	A	372	VAL
1	A	411	ASP
1	A	412	ASN
1	A	419	LEU
1	A	427	GLU
1	A	458	LYS
1	A	468	LEU
1	A	472	ILE
1	A	476	LEU
1	B	212	ARG
1	B	228	LEU
1	B	261	LYS
1	B	263	LYS
1	B	267	ILE
1	B	268	THR
1	B	311	LEU
1	B	318	LEU
1	B	335	ASN
1	B	351	GLU
1	B	355	SER
1	B	357	ARG
1	B	363	PHE
1	B	388	ILE
1	B	401	LEU
1	B	427	GLU
1	B	453	LEU
1	B	457	LYS
1	B	460	GLU
1	B	469	LEU
1	B	475	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	266	HIS
1	A	273	GLN
1	A	286	GLN
1	A	294	GLN
1	A	308	ASN

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Mol	Chain	Res	Type
1	A	323	HIS
1	A	402	ASN
1	A	410	GLN
1	A	412	ASN
1	A	424	ASN
1	A	425	HIS
1	A	430	GLN
1	A	449	HIS
1	A	454	GLN
1	A	470	GLN
1	B	217	HIS
1	B	308	ASN
1	B	335	ASN
1	B	410	GLN
1	B	412	ASN
1	B	420	GLN
1	B	437	GLN
1	B	444	GLN
1	B	449	HIS

### 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 ⓘ

There are no ligands in this entry.

### 5.7 Other polymers ⓘ

There are no such residues in this entry.



## 5.8 Polymer linkage issues ⓘ

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	270/286 (94%)	0.64	26 (9%)	10 16	34, 49, 79, 92	0
1	B	259/286 (90%)	0.63	24 (9%)	11 18	33, 48, 81, 86	0
All	All	529/572 (92%)	0.64	50 (9%)	10 17	33, 48, 79, 92	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	274	SER	9.4
1	A	274	SER	7.5
1	A	268	THR	6.1
1	A	269	PRO	6.1
1	A	266	HIS	5.5
1	A	476	LEU	5.5
1	B	461	THR	5.4
1	A	264	PHE	5.4
1	A	267	ILE	5.0
1	B	268	THR	4.3
1	B	243	ASP	4.3
1	A	263	LYS	3.8
1	A	360	PHE	3.6
1	B	264	PHE	3.5
1	B	256	MET	3.5
1	A	363	PHE	3.4
1	B	266	HIS	3.3
1	A	287	PHE	3.2
1	A	271	GLN	3.2
1	B	475	ASP	3.2
1	B	287	PHE	3.2
1	A	475	ASP	3.1
1	A	265	LYS	3.1
1	B	241	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	242	THR	2.8
1	A	426	PRO	2.7
1	A	241	THR	2.6
1	A	299	TYR	2.6
1	A	444	GLN	2.6
1	A	280	ARG	2.6
1	B	276	GLU	2.5
1	B	261	LYS	2.5
1	B	292	ALA	2.5
1	B	388	ILE	2.5
1	A	423	LEU	2.4
1	A	262	ILE	2.4
1	B	362	ASP	2.3
1	A	256	MET	2.3
1	B	279	ILE	2.3
1	B	352	PHE	2.3
1	B	263	LYS	2.3
1	A	358	LYS	2.3
1	B	459	THR	2.3
1	A	453	LEU	2.2
1	B	322	VAL	2.2
1	A	300	ALA	2.2
1	B	240	LYS	2.1
1	B	460	GLU	2.1
1	A	359	PRO	2.1
1	B	275	LYS	2.0

## 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 carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.