



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:46 AM UTC

PDB ID : 2ZK0 / pdb_00002zk0
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

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

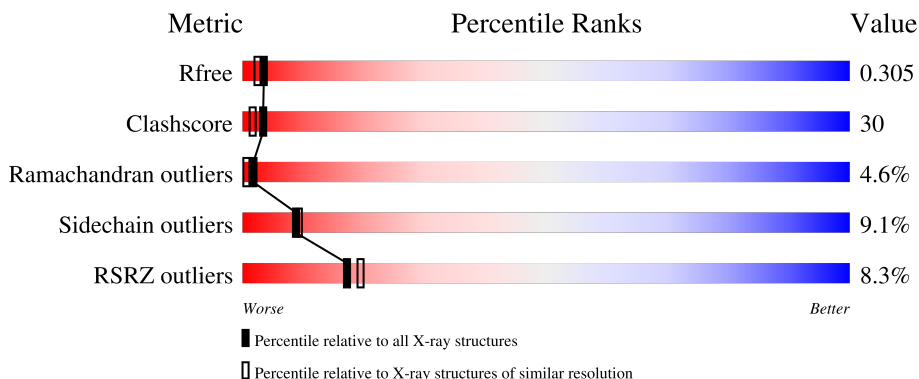
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.36 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}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	286	9% 50% 33% 10% 6%
1	B	286	7% 50% 31% 7% 9%

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

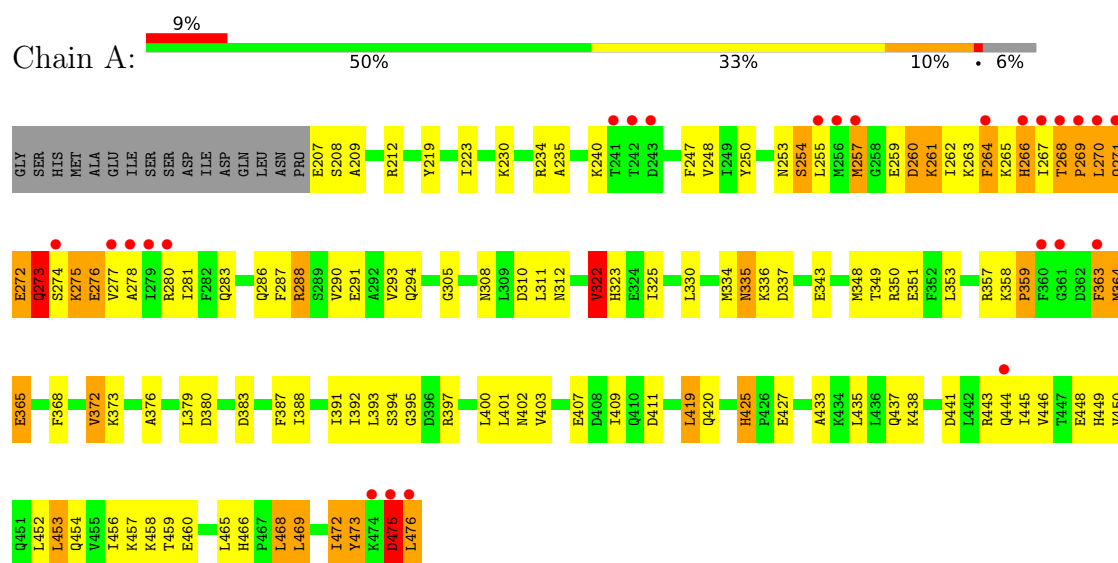
- Molecule 2 is water.

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

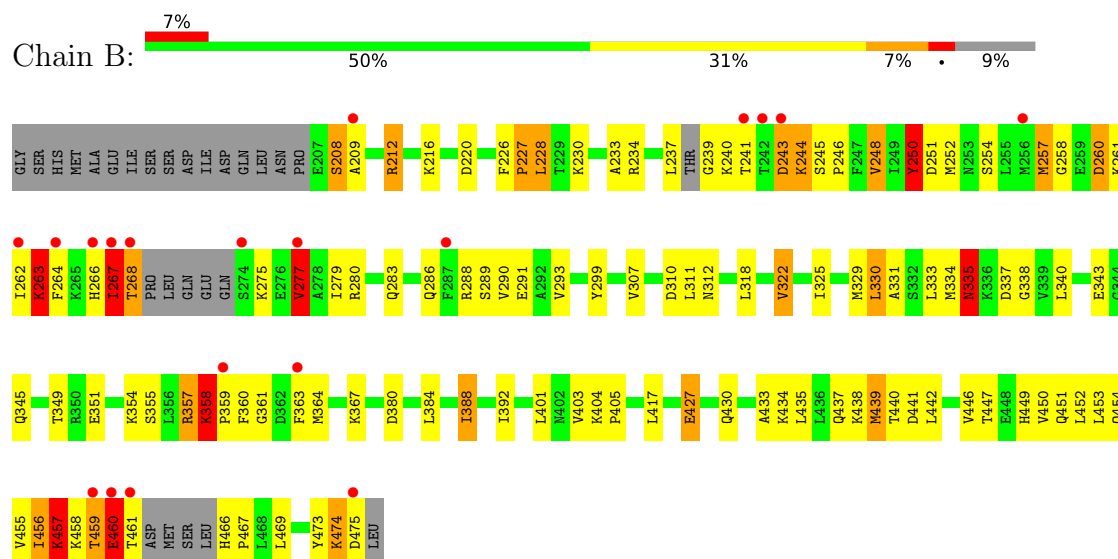
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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, α , β , γ	92.75Å 61.66Å 118.60Å 90.00° 102.69° 90.00°	Depositor
Resolution (Å)	32.77 – 2.36 32.77 – 2.36	Depositor EDS
% Data completeness (in resolution range)	92.9 (32.77-2.36) 92.9 (32.77-2.36)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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	1284 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å ²)	42.9	Xtriage
Anisotropy	0.541	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 33.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4303	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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	0.57	0/2203	1.12	15/2967 (0.5%)
1	B	0.55	0/2111	1.03	15/2838 (0.5%)
All	All	0.56	0/4314	1.08	30/5805 (0.5%)

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 (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	473	TYR	N-CA-C	12.95	129.22	113.16
1	A	275	LYS	N-CA-C	-12.51	89.50	109.39
1	A	475	ASP	N-CA-C	10.31	132.76	110.80
1	A	459	THR	N-CA-C	-7.92	102.25	112.23
1	B	257	MET	N-CA-C	-7.53	103.15	111.36
1	A	322	VAL	N-CA-C	7.52	118.05	110.23
1	B	403	VAL	N-CA-C	7.43	118.22	110.72
1	B	322	VAL	N-CA-C	7.35	117.47	110.42
1	B	263	LYS	N-CA-C	6.81	119.79	108.96
1	A	254	SER	N-CA-C	-6.69	103.99	111.28
1	B	277	VAL	N-CA-C	-6.59	104.06	110.72
1	A	288	ARG	N-CA-C	-6.42	104.36	111.36
1	A	425	HIS	CA-C-N	6.08	126.25	119.32
1	A	425	HIS	C-N-CA	6.08	126.25	119.32
1	A	268	THR	N-CA-C	-5.99	100.94	110.10
1	A	248	VAL	N-CA-C	5.90	116.79	108.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	248	VAL	N-CA-C	5.78	117.09	108.54
1	B	460	GLU	N-CA-C	-5.65	101.38	110.14
1	B	252	MET	N-CA-C	-5.54	105.24	111.28
1	A	364	MET	N-CA-C	5.38	119.01	112.23
1	B	267	ILE	N-CA-C	5.37	120.51	109.34
1	A	335	ASN	N-CA-C	-5.36	100.92	109.07
1	B	335	ASN	N-CA-C	-5.36	100.97	108.96
1	B	358	LYS	N-CA-C	5.31	121.54	109.81
1	B	459	THR	N-CA-C	-5.25	99.61	110.80
1	A	363	PHE	N-CA-C	5.24	116.80	111.14
1	A	247	PHE	N-CA-C	-5.22	101.95	110.20
1	B	208	SER	N-CA-C	-5.17	104.72	111.02
1	B	440	THR	N-CA-C	-5.15	105.30	112.45
1	B	250	TYR	N-CA-C	-5.09	106.20	114.09

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	142	0
1	B	2078	0	2142	119	0
2	A	26	0	0	2	0
2	B	33	0	0	1	0
All	All	4303	0	4374	260	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 30.

All (260) 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:C	1:B:335:ASN:HD22	1.80	0.90
1:B:335:ASN:ND2	1:B:337:ASP:H	1.72	0.88
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:B:330:LEU:HD22	1:B:334:MET:HE2	1.59	0.83
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:272:GLU:C	1:A:274:SER:H	1.89	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:274:SER:C	1:A:276:GLU:N	2.37	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:B:457:LYS:HZ3	1:B:461:THR:HA	1.47	0.76
1:A:267:ILE:HG13	1:A:283:GLN:HB2	1.68	0.76
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:HH11	1:B:212:ARG:CB	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:TYR:C	1:A:475:ASP:H	2.00	0.68
1:B:456:ILE:C	1:B:458:LYS:H	2.01	0.68
1:A:274:SER:C	1:A:276:GLU:H	2.00	0.68
1:A:272:GLU:HG3	1:A:274:SER:HB2	1.76	0.67
1:A:271:GLN:O	1:A:272:GLU:O	2.14	0.66
1:A:270:LEU:HB3	1:A:275:LYS:HB3	1.77	0.66
1:A:334:MET:HE2	1:A:368:PHE:CE1	2.31	0.66
1:B:251:ASP:HB2	1:B:254:SER:OG	1.97	0.65
1:A:273:GLN:O	1:A:273:GLN:HG2	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:212:ARG:HD3	1:A:419:LEU:HD13	1.80	0.63
1:B:241:THR:O	1:B:241:THR:HG22	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:331:ALA:HA	1:B:334:MET:HE3	1.81	0.62
1:B:457:LYS:NZ	1:B:457:LYS:HA	2.15	0.62
1:A:259:GLU:HG2	1:A:269:PRO:HD2	1.82	0.61
1:A:264:PHE:C	1:A:266:HIS:H	2.08	0.61
1:B:288:ARG:HD2	1:B:288:ARG:O	2.00	0.61
1:B:335:ASN:C	1:B:335:ASN:ND2	2.54	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:272:GLU:C	1:A:274:SER:N	2.54	0.60
1:A:207:GLU:HG3	1:A:209:ALA:H	1.65	0.60
1:A:257:MET:HE3	1:A:257:MET:HA	1.82	0.60
1:A:334:MET:HE2	1:A:368:PHE:CD1	2.36	0.60
1:A:268:THR:OG1	1:A:269:PRO:HD2	2.01	0.59
1:A:276:GLU:CD	1:A:357:ARG:HH21	2.09	0.59
1:B:335:ASN:HD22	1:B:337:ASP:H	1.44	0.59
1:A:293:VAL:HG22	1:A:322:VAL:CG1	2.33	0.59
1:A:468:LEU:O	1:A:472:ILE:HG22	2.01	0.59
1:B:330:LEU:HD22	1:B:334:MET:CE	2.31	0.59
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:A:379:LEU:HD11	1:A:435:LEU:HD13	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:TYR:C	1:A:475:ASP:N	2.63	0.56
1:B:212:ARG:HB3	1:B:212:ARG:NH1	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:263:LYS:HD2	1:B:263:LYS:C	2.31	0.56
1:B:264:PHE:HD2	1:B:266:HIS:CE1	2.23	0.56
1:B:333:LEU:HB3	1:B:340:LEU:HB2	1.87	0.56
1:B:335:ASN:ND2	1:B:337:ASP:N	2.49	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:311:LEU:HD13	1:A:311:LEU:C	2.31	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:A:437:GLN:OE1	1:B:439:MET:HE1	2.08	0.54
1:A:270:LEU:C	1:A:271:GLN:OE1	2.50	0.54
1:B:262:ILE:HG12	1:B:263:LYS:H	1.72	0.54
1:A:255:LEU:HD22	1:A:277:VAL:HG23	1.89	0.54
1:A:267:ILE:HG21	1:A:280:ARG:HA	1.90	0.54
1:B:457:LYS:HZ2	1:B:461:THR:HA	1.69	0.53
1:A:208:SER:HB2	1:A:419:LEU:HD11	1.90	0.53
1:B:359:PRO:HG2	1:B:360:PHE:CD2	2.42	0.53
1:A:365:GLU:OE1	1:A:365:GLU:HA	2.08	0.53
1:A:403:VAL:O	1:A:407:GLU:HG3	2.09	0.53
1:A:265:LYS:O	1:A:265:LYS:HG2	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:357:ARG:NH1	1:A:460:GLU:CD	2.68	0.52
1:A:401:LEU:C	1:A:402:ASN:HD22	2.18	0.52
1:A:272:GLU:CG	1:A:274:SER:HB2	2.40	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:251:ASP:H	1:B:254:SER:HB2	1.74	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:ASN:HD21	1:B:338:GLY:N	2.08	0.51
1:A:443:ARG:HG3	1:A:443:ARG:HH11	1.75	0.51
1:B:266:HIS:C	1:B:267:ILE:HG12	2.36	0.51
1:A:443:ARG:HG3	1:A:443:ARG:NH1	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:271:GLN:C	1:A:272:GLU:O	2.54	0.50
1:A:393:LEU:HD12	1:A:409:ILE:HB	1.93	0.50
1:A:466:HIS:CE1	1:A:468:LEU:HB2	2.46	0.49
1:B:358:LYS:HB3	1:B:359:PRO:CD	2.42	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:350:ARG:HG3	1:A:368:PHE:CD2	2.48	0.49
1:B:262:ILE:HD11	1:B:345:GLN:HB2	1.94	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:237:LEU:C	1:B:239:GLY:N	2.71	0.48
1:B:289:SER:O	1:B:293:VAL:HG23	2.13	0.48
1:A:212:ARG:HH12	1:A:420:GLN:HA	1.78	0.48
1:A:266:HIS:CD2	1:A:287:PHE:CB	2.97	0.48
1:B:330:LEU:O	1:B:334:MET:HG3	2.14	0.48
1:B:456:ILE:C	1:B:458:LYS:N	2.62	0.48
1:A:325:ILE:HD11	1:A:392:ILE:CG1	2.44	0.48
1:B:208:SER:O	1:B:209:ALA:C	2.57	0.47
1:B:243:ASP:CG	1:B:244:LYS:HZ1	2.20	0.47
1:A:363:PHE:CE1	1:A:452:LEU:HB2	2.50	0.47
1:B:473:TYR:O	1:B:474:LYS:O	2.33	0.47
1:A:291:GLU:HA	1:A:294:GLN:NE2	2.29	0.47
1:B:367:LYS:HZ1	1:B:449:HIS:CD2	2.32	0.47
1:B:267:ILE:C	1:B:268:THR:HG22	2.40	0.47
1:A:270:LEU:C	1:A:271:GLN:CG	2.87	0.47
1:B:288:ARG:HH11	1:B:291:GLU:HB2	1.80	0.47
1:A:266:HIS:CE1	1:A:291:GLU:OE2	2.67	0.47
1:A:270:LEU:O	1:A:275:LYS:CB	2.59	0.47
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:PHE:CG	1:B:329:MET:HE1	2.50	0.46
1:B:234:ARG:O	1:B:239:GLY:HA3	2.15	0.46
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:343:GLU:OE2	1:B:343:GLU:N	2.48	0.46
1:B:367:LYS:NZ	1:B:449:HIS:HD2	2.13	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: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:357:ARG:HH11	1:B:357:ARG:CG	2.28	0.46
1:A:322:VAL:HG12	1:A:323:HIS:N	2.30	0.46
1:B:457:LYS:HG3	1:B:461:THR:HG23	1.98	0.46
1:A:290:VAL:HG21	1:A:466:HIS:CD2	2.51	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:250:TYR:CE2	1:A:254:SER:OG	2.69	0.46
1:B:257:MET:O	1:B:260:ASP:HB3	2.15	0.46
1:B:358:LYS:CB	1:B:359:PRO:CD	2.93	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: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:A:310:ASP:OD2	1:A:312:ASN:HB2	2.16	0.45
1:B:330:LEU:HD22	1:B:334:MET:SD	2.56	0.45
1:B:335:ASN:HD22	1:B:337:ASP:N	2.13	0.45
1:A:276:GLU:HG3	1:A:357:ARG:HH21	1.82	0.45
1:A:262:ILE:HG22	1:A:264:PHE:CD1	2.51	0.45
1:A:273:GLN:O	1:A:276:GLU:CA	2.48	0.45
1:B:457:LYS:HZ3	1:B:457:LYS:HA	1.80	0.45
1:A:472:ILE:HG12	1:A:472:ILE:O	2.16	0.45
1:A:259:GLU:HA	1:A:264:PHE:CZ	2.52	0.44
1:A:330:LEU:HD21	1:A:364:MET:HE1	1.99	0.44
1:A:357:ARG:O	1:A:359:PRO:N	2.50	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:250:TYR:HB3	1:B:349:THR:HG21	2.00	0.44
1:B:358:LYS:HB3	1:B:359:PRO:HD3	1.99	0.44
1:A:270:LEU:C	1:A:271:GLN:HG2	2.42	0.44
1:B:310:ASP:OD1	1:B:312:ASN:N	2.51	0.44
1:B:473:TYR:O	1:B:474:LYS:C	2.59	0.44

Continued on next page...

Continued from previous page...

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:A:435:LEU:O	1:A:438:LYS:HB2	2.18	0.43
1:B:208:SER:OG	1:B:209:ALA:N	2.51	0.43
1:B:286:GLN:O	1:B:289:SER:HB2	2.18	0.43
1:B:325:ILE:HD11	1:B:392:ILE:HG13	2.00	0.43
1:A:276:GLU:O	1:A:277:VAL:C	2.59	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:A:260:ASP:O	1:A:261:LYS:C	2.62	0.43
1:A:264:PHE:C	1:A:266:HIS:N	2.76	0.43
1:B:262:ILE:HG12	1:B:263:LYS:N	2.34	0.43
1:A:219:TYR:CZ	1:A:223:ILE:HD11	2.54	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:HA	1:A:454:GLN:NE2	2.35	0.42
1:A:472:ILE:O	1:A:475:ASP:OD2	2.38	0.42
1:B:260:ASP:O	1:B:261:LYS:C	2.62	0.42
1:B:330:LEU:CD2	1:B:334:MET:HE2	2.41	0.42
1:A:212:ARG:CD	1:A:419:LEU:HD13	2.49	0.42
1:A:380:ASP:C	1:A:380:ASP:OD1	2.62	0.42
1:A:388:ILE:HD13	1:A:391:ILE:HD12	2.01	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:244:LYS:O	1:B:245:SER:C	2.63	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:H	1:A:261:LYS:HD2	1.85	0.42
1:B:451:GLN:O	1:B:454:GLN:HB3	2.19	0.42
1:B:451:GLN:HA	1:B:451:GLN:OE1	2.21	0.41
1:A:273:GLN:H	1:A:273:GLN:NE2	2.17	0.41
1:A:283:GLN:O	1:A:286:GLN:HB2	2.20	0.41
1:A:472:ILE:HD13	1:A:472:ILE:C	2.45	0.41
1:B:447:THR:O	1:B:450:VAL:HG22	2.21	0.41
1:A:456:ILE:C	1:A:458:LYS:N	2.79	0.41
1:B:226:PHE:HA	1:B:227:PRO:HD3	1.90	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:ASN:O	1:A:337:ASP:N	2.54	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:264:PHE:O	1:A:266:HIS:N	2.52	0.41
1:B:354:LYS:HA	1:B:361:GLY:O	2.21	0.40
1:B:380:ASP:OD1	1:B:380:ASP:C	2.65	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:299:TYR:HD2	1:B:388:ILE:HD11	1.86	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:O	1:B:266:HIS:ND1	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%)	2	1
1	B	251/286 (88%)	226 (90%)	13 (5%)	12 (5%)	2	0
All	All	519/572 (91%)	472 (91%)	23 (4%)	24 (5%)	2	0

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	358	LYS
1	B	457	LYS
1	B	474	LYS
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%)	11	12
1	B	232/257 (90%)	208 (90%)	24 (10%)	7	6
All	All	475/514 (92%)	432 (91%)	43 (9%)	9	9

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	253	ASN
1	A	257	MET
1	A	263	LYS
1	A	264	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	270	LEU
1	A	271	GLN
1	A	273	GLN
1	A	322	VAL
1	A	343	GLU
1	A	365	GLU
1	A	372	VAL
1	A	411	ASP
1	A	419	LEU
1	A	427	GLU
1	A	453	LEU
1	A	468	LEU
1	A	469	LEU
1	A	472	ILE
1	A	476	LEU
1	B	212	ARG
1	B	228	LEU
1	B	263	LYS
1	B	267	ILE
1	B	268	THR
1	B	277	VAL
1	B	311	LEU
1	B	318	LEU
1	B	322	VAL
1	B	330	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	439	MET
1	B	453	LEU
1	B	457	LYS
1	B	460	GLU
1	B	469	LEU
1	B	475	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	273	GLN
1	A	283	GLN
1	A	286	GLN
1	A	294	GLN
1	A	308	ASN
1	A	323	HIS
1	A	402	ASN
1	A	410	GLN
1	A	412	ASN
1	A	425	HIS
1	A	430	GLN
1	A	454	GLN
1	A	470	GLN
1	B	217	HIS
1	B	308	ASN
1	B	335	ASN
1	B	345	GLN
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 [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

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, 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	270/286 (94%)	0.67	25 (9%) 14 17	34, 49, 79, 92	0
1	B	259/286 (90%)	0.61	19 (7%) 21 24	33, 48, 81, 86	0
All	All	529/572 (92%)	0.64	44 (8%) 17 19	33, 48, 79, 92	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	274	SER	4.7
1	B	266	HIS	4.6
1	B	459	THR	4.3
1	A	363	PHE	4.0
1	A	269	PRO	3.9
1	B	267	ILE	3.9
1	B	461	THR	3.8
1	A	270	LEU	3.6
1	B	264	PHE	3.6
1	B	274	SER	3.6
1	A	476	LEU	3.2
1	A	241	THR	3.2
1	A	255	LEU	3.2
1	B	475	ASP	3.1
1	A	268	THR	3.0
1	B	242	THR	3.0
1	A	271	GLN	3.0
1	A	475	ASP	3.0
1	B	262	ILE	3.0
1	B	268	THR	2.9
1	A	360	PHE	2.9
1	A	266	HIS	2.8
1	B	359	PRO	2.7
1	B	287	PHE	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	280	ARG	2.6
1	B	209	ALA	2.6
1	B	363	PHE	2.6
1	A	267	ILE	2.6
1	A	242	THR	2.6
1	A	243	ASP	2.5
1	B	460	GLU	2.5
1	A	444	GLN	2.5
1	B	241	THR	2.5
1	A	361	GLY	2.5
1	A	256	MET	2.4
1	A	474	LYS	2.3
1	A	264	PHE	2.3
1	A	278	ALA	2.3
1	B	243	ASP	2.2
1	A	277	VAL	2.2
1	B	256	MET	2.2
1	B	277	VAL	2.1
1	A	279	ILE	2.1
1	A	257	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 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.