



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 03:32 PM GMT

PDB ID : 3B9N  
Title : Crystal structure of long-chain alkane monooxygenase (LadA)  
Authors : Li, L.; Yang, W.; Xu, F.; Bartlam, M.; Rao, Z.  
Deposited on : 2007-11-06  
Resolution : 2.70 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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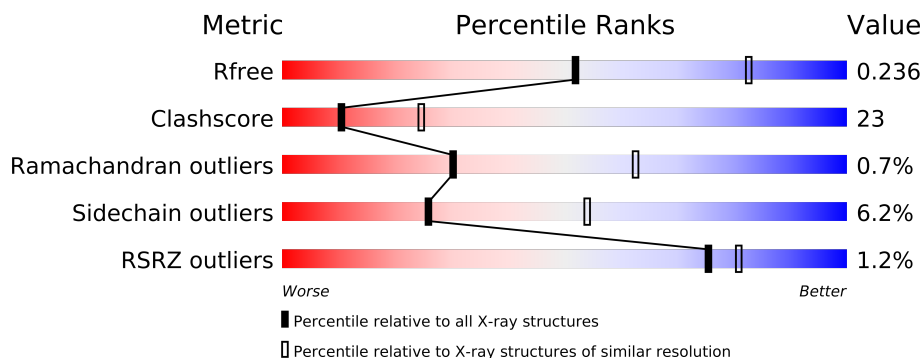
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance



The reported resolution of this entry is 2.70 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))
$R_{free}$	66092	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	440	
1	B	440	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7369 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Alkane monooxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	433	Total	C	N	O	S	0	0	0
			3513	2243	609	647	14			
1	B	434	Total	C	N	O	S	0	0	0
			3520	2248	609	648	15			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	172	Total	O	0	0
			172	172		
2	B	164	Total	O	0	0
			164	164		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.50Å 77.50Å 323.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 48.86 – 2.67	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.70) 70.9 (48.86-2.67)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	19.30 (at 2.69Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.183 , 0.249 0.184 , 0.236	Depositor DCC
$R_{free}$ test set	1999 reflections (9.81%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.8	Xtriage
Anisotropy	0.846	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 19.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 22129 reflections (0.005%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7369	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.92 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.4297e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

## 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	0.37	0/3606	0.62	1/4877 (0.0%)
1	B	0.36	0/3613	0.61	0/4886
All	All	0.37	0/7219	0.62	1/9763 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	136	THR	N-CA-C	-5.49	96.17	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3513	0	3410	168	0
1	B	3520	0	3423	162	0
2	A	172	0	0	10	0
2	B	164	0	0	11	0
All	All	7369	0	6833	322	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 23.

All (322) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:332:ILE:HD11	1:B:336:GLU:HB2	1.48	0.95
1:B:45:LEU:HD12	1:B:48:LYS:HE3	1.45	0.95
1:A:422:TYR:HD1	1:A:423:ARG:HG3	1.40	0.87
1:A:53:ALA:HB2	1:A:100:ALA:HB3	1.59	0.84
1:A:380:TYR:H	1:A:385:THR:HG21	1.46	0.81
1:A:285:VAL:HG12	1:A:359:VAL:HG21	1.65	0.79
1:A:219:GLN:NE2	1:A:413:ARG:H	1.81	0.78
1:B:332:ILE:HD13	1:B:333:SER:N	1.97	0.78
1:A:29:GLN:NE2	1:A:32:ARG:HH11	1.81	0.78
1:A:324:SER:HB3	1:A:327:ASP:OD1	1.84	0.77
1:A:144:LYS:HG2	1:B:209:PRO:HG2	1.67	0.76
1:B:234:ARG:HD2	1:B:260:ASP:OD1	1.85	0.76
1:A:226:GLN:HB2	1:A:241:ALA:HB2	1.68	0.76
1:A:150:LYS:HD2	1:A:150:LYS:O	1.85	0.76
1:A:28:ASN:ND2	1:A:382:SER:H	1.84	0.75
1:A:239:LYS:HG2	1:A:429:ILE:HD11	1.67	0.75
1:A:117:ARG:HG3	1:A:214:CYS:SG	2.27	0.74
1:B:267:LYS:HB3	2:B:571:HOH:O	1.86	0.73
1:A:422:TYR:CD1	1:A:423:ARG:HG3	2.24	0.72
1:A:149:LYS:HD3	1:A:149:LYS:H	1.53	0.72
1:A:345:ASP:HB3	1:A:351:LEU:HD23	1.72	0.72
1:B:275:ILE:HG22	1:B:277:MET:HE3	1.72	0.72
1:B:318:TYR:CG	1:B:329:ILE:HD11	2.25	0.71
1:B:275:ILE:HG22	1:B:277:MET:CE	2.20	0.71
1:A:296:LEU:HD12	1:A:353:VAL:HG21	1.73	0.70
1:B:258:VAL:HG13	1:B:277:MET:HG3	1.74	0.70
1:A:336:GLU:HG2	1:A:340:ASN:ND2	2.07	0.69
1:A:285:VAL:CG1	1:A:359:VAL:HG21	2.21	0.69
1:B:28:ASN:ND2	1:B:382:SER:H	1.90	0.69
1:B:267:LYS:HE2	2:B:571:HOH:O	1.93	0.68
1:A:29:GLN:HE22	1:A:32:ARG:HH11	1.40	0.67
1:B:226:GLN:NE2	1:B:228:GLY:H	1.92	0.67
1:B:324:SER:HB3	1:B:327:ASP:OD1	1.94	0.66
1:B:53:ALA:HB2	1:B:100:ALA:HB3	1.78	0.66
1:B:226:GLN:HE22	1:B:228:GLY:N	1.93	0.66
1:B:332:ILE:CD1	1:B:336:GLU:HB2	2.23	0.65
1:B:28:ASN:HD22	1:B:29:GLN:H	1.45	0.65
1:A:106:SER:HA	1:A:135:VAL:O	1.97	0.65
1:B:106:SER:HA	1:B:135:VAL:O	1.97	0.65
1:A:340:ASN:HA	1:A:343:LYS:CD	2.26	0.65
1:B:226:GLN:HE22	1:B:228:GLY:H	1.43	0.64
1:B:276:LYS:HA	1:B:373:ASP:OD1	1.97	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:2:THR:HG23	1:B:3:LYS:NZ	2.12	0.64
1:A:217:SER:HB2	1:A:218:PRO:HD2	1.80	0.64
1:A:138:HIS:CD2	1:A:139:LEU:H	2.16	0.64
1:B:40:THR:O	1:B:44:GLN:HG3	1.98	0.64
1:A:219:GLN:HE21	1:A:413:ARG:H	1.45	0.63
1:A:149:LYS:CD	1:A:149:LYS:H	2.07	0.63
1:A:166:GLU:HG2	1:A:170:LYS:HE3	1.81	0.62
1:A:267:LYS:HB2	2:A:514:HOH:O	1.99	0.62
1:B:17:HIS:CD2	1:B:18:ILE:HD12	2.34	0.62
1:B:33:TYR:CE2	1:B:34:THR:HG23	2.35	0.62
1:A:80:ILE:HD11	2:B:654:HOH:O	2.00	0.62
1:A:306:GLU:HB2	2:A:566:HOH:O	2.00	0.61
1:B:2:THR:HG23	1:B:3:LYS:HZ3	1.65	0.61
1:B:305:LEU:O	1:B:309:LEU:HD23	2.01	0.61
1:B:226:GLN:HB2	1:B:241:ALA:HB2	1.81	0.61
1:B:181:VAL:HG21	1:B:215:GLU:OE1	2.00	0.61
1:B:422:TYR:HD1	1:B:423:ARG:HG3	1.65	0.61
1:B:183:ARG:HG2	1:B:190:TYR:CE1	2.36	0.60
1:B:79:GLN:O	1:B:82:VAL:HG22	2.02	0.60
1:A:168:CYS:HB3	1:A:172:TRP:CZ3	2.36	0.60
1:A:410:GLY:O	1:A:415:LYS:NZ	2.35	0.59
1:A:149:LYS:HD3	1:A:149:LYS:N	2.16	0.59
1:B:329:ILE:CG2	1:B:337:ILE:HD12	2.32	0.59
1:A:239:LYS:CG	1:A:429:ILE:HD11	2.32	0.59
1:B:271:ASN:OD1	1:B:273:ASP:HB2	2.03	0.59
1:A:356:PRO:HG3	1:A:392:LEU:HB3	1.83	0.59
1:A:244:VAL:HG11	1:A:261:ILE:HD13	1.83	0.59
1:A:12:MET:HE3	1:A:57:ALA:HB3	1.83	0.59
1:B:282:CYS:HB2	1:B:349:PHE:CE2	2.38	0.59
1:B:282:CYS:HB2	1:B:349:PHE:HE2	1.68	0.58
1:B:117:ARG:HG3	1:B:214:CYS:SG	2.43	0.58
1:B:405:VAL:HG23	1:B:406:ASP:OD1	2.03	0.58
1:B:278:PHE:HA	1:B:374:GLY:O	2.04	0.58
1:A:105:PHE:HB3	1:A:132:TRP:NE1	2.19	0.58
1:A:67:ARG:HH11	1:A:67:ARG:HG3	1.67	0.58
1:B:134:VAL:HG11	1:B:165:LEU:HD21	1.84	0.58
1:A:9:ALA:HB1	1:A:386:PHE:CZ	2.38	0.58
1:B:166:GLU:HG2	1:B:170:LYS:HE3	1.85	0.58
1:A:340:ASN:HA	1:A:343:LYS:HD2	1.86	0.57
1:A:153:GLU:O	1:A:157:ARG:HG3	2.05	0.57
1:A:28:ASN:ND2	1:A:29:GLN:H	2.02	0.57
1:A:209:PRO:HD2	1:B:145:ASN:OD1	2.05	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:137:SER:O	1:A:157:ARG:NH1	2.36	0.56
1:B:137:SER:O	1:B:157:ARG:NH1	2.38	0.56
1:B:28:ASN:ND2	1:B:29:GLN:H	2.03	0.56
2:A:594:HOH:O	1:B:110:GLU:HG2	2.06	0.56
1:B:296:LEU:O	1:B:296:LEU:HD23	2.05	0.56
1:B:332:ILE:HD13	1:B:333:SER:H	1.68	0.56
1:A:17:HIS:CD2	1:A:18:ILE:HD12	2.41	0.56
1:A:133:ASN:HA	1:A:225:TYR:HB2	1.86	0.56
1:B:198:GLU:HB3	1:B:209:PRO:O	2.06	0.56
1:A:381:VAL:HG13	1:A:384:GLY:HA3	1.88	0.56
1:A:223:VAL:HA	1:A:242:GLU:OE2	2.06	0.55
1:B:434:ARG:HG2	2:B:656:HOH:O	2.05	0.55
1:B:329:ILE:HG21	1:B:337:ILE:HD12	1.88	0.55
1:A:70:ARG:HD3	2:A:458:HOH:O	2.06	0.55
1:B:186:GLU:H	1:B:186:GLU:CD	2.09	0.55
1:A:287:LYS:NZ	1:A:287:LYS:HB3	2.21	0.55
1:B:277:MET:HA	1:B:277:MET:HE2	1.88	0.54
1:A:270:ARG:HD2	2:A:474:HOH:O	2.07	0.54
1:A:19:ALA:HB2	1:A:380:TYR:CD1	2.43	0.54
1:B:379:GLN:NE2	1:B:382:SER:OG	2.41	0.54
1:B:45:LEU:O	1:B:48:LYS:HG3	2.07	0.54
1:B:182:ILE:HD11	1:B:189:ILE:CG2	2.38	0.54
1:B:111:HIS:CD2	1:B:113:TYR:H	2.25	0.53
1:B:359:VAL:HG12	1:B:363:MET:CE	2.38	0.53
1:B:359:VAL:HG12	1:B:363:MET:HE2	1.89	0.53
1:B:285:VAL:HG21	1:B:393:VAL:CG2	2.39	0.53
1:A:138:HIS:CD2	1:A:139:LEU:HG	2.43	0.53
1:A:138:HIS:CG	1:A:139:LEU:H	2.27	0.53
1:A:263:LYS:HA	1:A:266:LYS:HD3	1.91	0.53
1:A:329:ILE:HG22	1:A:330:GLY:N	2.23	0.53
1:B:381:VAL:HG13	1:B:384:GLY:HA3	1.91	0.52
1:A:367:VAL:HA	1:A:372:ILE:HG12	1.91	0.52
1:A:413:ARG:NH1	1:A:424:LEU:HD13	2.24	0.52
1:B:3:LYS:O	1:B:3:LYS:HD2	2.09	0.52
1:A:151:ILE:HD12	1:A:151:ILE:N	2.24	0.52
1:B:363:MET:CE	1:B:393:VAL:HG11	2.39	0.52
1:B:111:HIS:HD2	1:B:113:TYR:H	1.57	0.52
1:B:51:PHE:HE1	1:B:390:ILE:HG12	1.75	0.52
1:A:239:LYS:HG2	1:A:429:ILE:CD1	2.36	0.52
1:A:340:ASN:HA	1:A:343:LYS:HD3	1.91	0.52
1:B:242:GLU:OE1	1:B:413:ARG:HD3	2.10	0.52
1:B:329:ILE:O	1:B:329:ILE:HG12	2.09	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:413:ARG:HG2	1:A:421:ASN:O	2.09	0.52
1:B:107:THR:HB	1:B:164:TYR:CD1	2.44	0.51
1:A:258:VAL:HG13	1:A:277:MET:HG3	1.92	0.51
1:B:112:PRO:HG3	1:B:164:TYR:CE1	2.45	0.51
1:A:244:VAL:HB	1:A:277:MET:HE2	1.92	0.51
1:A:312:TYR:CE1	1:A:316:THR:HG21	2.46	0.51
1:B:197:HIS:O	1:B:211:PRO:HB3	2.11	0.51
1:A:79:GLN:O	1:A:82:VAL:HG22	2.11	0.51
1:A:28:ASN:HD21	1:A:382:SER:H	1.59	0.51
1:A:254:LEU:O	1:A:258:VAL:HG23	2.11	0.51
1:A:300:GLN:OE1	1:A:344:LEU:HD12	2.10	0.51
1:A:22:LEU:HD23	1:A:380:TYR:O	2.11	0.50
1:B:413:ARG:HG2	1:B:421:ASN:O	2.10	0.50
1:B:300:GLN:NE2	1:B:344:LEU:HD13	2.26	0.50
1:A:393:VAL:HG12	1:A:397:LEU:HD22	1.93	0.50
1:A:198:GLU:HB3	1:A:209:PRO:O	2.11	0.50
1:A:296:LEU:O	1:A:296:LEU:HD23	2.11	0.50
1:A:144:LYS:CG	1:B:209:PRO:HG2	2.39	0.50
1:A:336:GLU:HG2	1:A:340:ASN:HD21	1.76	0.50
1:B:271:ASN:HB3	1:B:274:HIS:CD2	2.47	0.50
1:B:428:HIS:CE1	1:B:429:ILE:HD12	2.47	0.50
1:B:123:ASP:OD1	1:B:128:GLY:HA2	2.12	0.50
1:B:45:LEU:HD12	1:B:48:LYS:CE	2.30	0.50
1:B:178:ASP:HA	1:B:220:ARG:HH21	1.77	0.50
1:A:42:LEU:O	1:A:46:LEU:HG	2.11	0.50
1:B:340:ASN:HA	1:B:343:LYS:HE2	1.94	0.50
1:B:11:GLU:HB2	1:B:54:LEU:HD21	1.93	0.50
1:B:305:LEU:HD13	1:B:309:LEU:HD23	1.93	0.49
1:A:252:GLU:H	1:A:252:GLU:CD	2.15	0.49
1:A:25:HIS:CD2	1:A:27:GLU:H	2.29	0.49
1:B:219:GLN:NE2	1:B:413:ARG:H	2.10	0.49
1:B:296:LEU:HD12	1:B:353:VAL:HG11	1.94	0.49
1:B:9:ALA:HB1	1:B:386:PHE:CZ	2.47	0.49
1:A:138:HIS:O	1:A:139:LEU:C	2.51	0.49
1:B:219:GLN:HE21	1:B:413:ARG:H	1.59	0.49
1:A:225:TYR:HH	1:A:412:TYR:HH	1.59	0.49
1:A:226:GLN:HE22	1:A:228:GLY:H	1.60	0.49
1:A:217:SER:HB2	1:A:218:PRO:CD	2.42	0.49
1:A:167:VAL:HG22	1:A:201:HIS:CD2	2.47	0.49
1:A:29:GLN:NE2	1:A:32:ARG:HD3	2.28	0.49
1:A:66:TYR:CZ	1:A:309:LEU:HD23	2.48	0.49
1:A:197:HIS:O	1:A:211:PRO:HB3	2.13	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:244:VAL:HG11	1:A:261:ILE:CD1	2.43	0.49
1:B:332:ILE:HD11	1:B:336:GLU:CB	2.31	0.48
1:A:285:VAL:HG11	1:A:393:VAL:CG2	2.43	0.48
1:A:29:GLN:HE21	1:A:32:ARG:HD3	1.78	0.48
1:A:277:MET:HE2	1:A:277:MET:HA	1.95	0.48
1:A:163:GLU:O	1:A:167:VAL:HG23	2.14	0.48
1:A:50:LYS:HA	1:A:407:TYR:CZ	2.49	0.48
1:B:289:HIS:HE1	2:B:587:HOH:O	1.96	0.48
1:B:249:LYS:HB3	1:B:349:PHE:C	2.34	0.48
1:B:80:ILE:HA	1:B:81:PRO:C	2.33	0.48
1:B:262:ARG:NH1	1:B:272:PRO:O	2.46	0.47
1:A:53:ALA:HA	1:A:99:LEU:HD22	1.97	0.47
1:B:217:SER:HB2	1:B:218:PRO:HD2	1.95	0.47
1:A:18:ILE:HG22	1:A:19:ALA:N	2.29	0.47
1:B:275:ILE:HG22	1:B:277:MET:HE1	1.93	0.47
1:A:226:GLN:HE22	1:A:228:GLY:N	2.13	0.47
1:B:244:VAL:HB	1:B:277:MET:HE2	1.95	0.47
1:A:166:GLU:CG	1:A:170:LYS:HE3	2.45	0.47
1:A:55:PHE:CD2	1:A:55:PHE:C	2.88	0.47
1:A:363:MET:CE	1:A:393:VAL:HG11	2.44	0.47
1:A:363:MET:HE1	1:A:393:VAL:HG11	1.96	0.47
1:B:112:PRO:HG3	1:B:164:TYR:CD1	2.50	0.47
1:B:332:ILE:HG23	1:B:337:ILE:HG13	1.96	0.46
1:B:17:HIS:CG	1:B:18:ILE:HD12	2.51	0.46
1:A:286:GLY:O	1:A:356:PRO:HD3	2.15	0.46
1:A:204:LYS:NZ	2:A:545:HOH:O	2.46	0.46
1:A:364:GLN:O	1:A:368:GLU:HG3	2.15	0.46
1:A:11:GLU:HB3	1:A:54:LEU:HD21	1.97	0.46
1:A:208:VAL:HA	1:A:209:PRO:HD3	1.73	0.46
1:A:424:LEU:HA	1:A:425:PRO:HD3	1.76	0.46
1:A:287:LYS:HZ3	1:A:287:LYS:HB3	1.79	0.46
1:A:312:TYR:HE2	1:A:320:LEU:HD21	1.79	0.46
1:A:89:ILE:HD12	1:A:101:PHE:HB3	1.97	0.46
1:B:53:ALA:HA	1:B:99:LEU:HD22	1.98	0.46
1:B:386:PHE:O	1:B:390:ILE:HG13	2.16	0.46
1:B:413:ARG:CZ	1:B:424:LEU:HD13	2.45	0.46
1:B:424:LEU:HD23	1:B:430:ALA:HB3	1.97	0.46
1:B:59:VAL:HG23	1:B:59:VAL:O	2.16	0.46
1:B:390:ILE:HA	1:B:394:VAL:CG2	2.46	0.46
1:B:66:TYR:O	1:B:67:ARG:HB2	2.16	0.46
1:A:118:ARG:HD3	1:B:87:MET:HE3	1.97	0.46
1:B:41:GLU:HG3	2:B:552:HOH:O	2.16	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:57:ALA:HA	1:A:104:THR:OG1	2.16	0.45
1:B:86:LEU:CD1	1:B:103:VAL:HG21	2.46	0.45
1:A:345:ASP:HB3	1:A:351:LEU:CD2	2.44	0.45
1:B:283:VAL:CG1	1:B:285:VAL:HG22	2.47	0.45
1:A:396:GLU:O	1:A:400:ARG:HG3	2.16	0.45
1:B:44:GLN:HG2	1:B:95:VAL:HG13	1.97	0.45
1:B:414:GLU:O	1:B:418:GLY:N	2.46	0.45
1:A:226:GLN:NE2	1:A:228:GLY:H	2.14	0.45
1:B:182:ILE:O	1:B:183:ARG:C	2.56	0.45
1:B:24:ARG:NH1	2:B:578:HOH:O	2.48	0.44
1:A:296:LEU:CD1	1:A:353:VAL:HG21	2.45	0.44
2:A:441:HOH:O	1:B:215:GLU:HG2	2.17	0.44
1:B:219:GLN:O	1:B:221:THR:N	2.48	0.44
1:B:101:PHE:O	1:B:130:ILE:HD12	2.16	0.44
1:B:410:GLY:O	1:B:415:LYS:NZ	2.49	0.44
1:A:20:HIS:HE1	1:A:311:HIS:ND1	2.15	0.44
1:B:139:LEU:HA	1:B:140:PRO:HD3	1.77	0.44
1:A:182:ILE:HD11	1:A:189:ILE:CG2	2.48	0.44
1:A:242:GLU:OE1	1:A:413:ARG:HD3	2.18	0.44
1:B:226:GLN:HE22	1:B:228:GLY:CA	2.29	0.44
1:A:414:GLU:O	1:A:418:GLY:N	2.45	0.44
1:A:362:GLU:O	1:A:366:LEU:HD22	2.16	0.44
1:B:86:LEU:HD21	1:B:119:MET:CE	2.48	0.44
1:B:323:TYR:HB3	1:B:334:VAL:HG21	2.00	0.44
1:A:381:VAL:O	1:A:385:THR:HG23	2.18	0.44
1:B:309:LEU:HD12	1:B:320:LEU:HB2	1.97	0.44
1:B:79:GLN:O	1:B:82:VAL:CG2	2.65	0.44
1:A:76:GLU:OE2	1:B:188:ASN:ND2	2.51	0.44
1:A:73:ALA:O	1:A:77:ALA:N	2.50	0.44
1:A:102:ALA:HA	1:A:131:ALA:HB3	2.00	0.44
1:A:22:LEU:CD2	1:A:380:TYR:O	2.65	0.44
1:B:220:ARG:HD2	1:B:423:ARG:HD3	2.00	0.44
1:A:219:GLN:O	1:A:221:THR:N	2.50	0.44
1:B:356:PRO:HB3	1:B:392:LEU:O	2.18	0.43
1:A:215:GLU:HG2	2:B:548:HOH:O	2.18	0.43
1:B:305:LEU:HD13	1:B:309:LEU:CD2	2.48	0.43
1:A:277:MET:HA	1:A:277:MET:CE	2.48	0.43
1:A:204:LYS:HD3	1:A:205:TYR:CE2	2.53	0.43
1:A:67:ARG:HG3	1:A:67:ARG:NH1	2.32	0.43
1:A:14:CYS:HB3	1:A:82:VAL:HG13	1.99	0.43
1:B:409:GLU:OE1	1:B:409:GLU:N	2.51	0.43
1:B:135:VAL:HG13	1:B:136:THR:O	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:363:MET:HE2	1:B:393:VAL:HG11	2.01	0.43
1:A:111:HIS:CG	1:A:112:PRO:HD2	2.53	0.43
1:A:106:SER:HA	1:A:135:VAL:HG12	2.01	0.43
1:B:151:ILE:HG23	1:B:157:ARG:HH21	1.84	0.43
1:B:22:LEU:HD23	1:B:380:TYR:O	2.19	0.43
1:B:394:VAL:HB	1:B:395:PRO:HD3	2.00	0.43
1:B:281:ILE:HG22	1:B:375:PHE:HB3	2.01	0.43
1:B:347:LYS:HA	1:B:347:LYS:HE3	2.01	0.43
1:A:323:TYR:HB3	1:A:334:VAL:HG21	2.00	0.43
1:A:300:GLN:CA	1:A:344:LEU:HD11	2.49	0.43
1:A:332:ILE:CG2	1:A:336:GLU:HB3	2.48	0.43
1:B:182:ILE:HD11	1:B:189:ILE:HG22	1.99	0.43
1:B:242:GLU:OE2	1:B:413:ARG:NH1	2.51	0.43
1:A:165:LEU:HD12	1:A:240:HIS:CG	2.54	0.43
1:B:86:LEU:HD12	1:B:103:VAL:HG21	2.01	0.42
1:B:259:ASP:O	1:B:263:LYS:HG2	2.18	0.42
1:A:100:ALA:HA	1:A:129:ARG:HB3	2.00	0.42
1:A:400:ARG:HB2	1:A:402:LEU:HD12	2.00	0.42
1:A:102:ALA:HA	1:A:131:ALA:O	2.20	0.42
1:B:28:ASN:HD22	1:B:29:GLN:N	2.13	0.42
1:A:275:ILE:HG22	1:A:277:MET:HE3	2.01	0.42
1:A:44:GLN:HG3	1:A:95:VAL:HG11	2.00	0.42
1:A:80:ILE:HG23	1:A:80:ILE:O	2.20	0.42
1:B:5:ILE:HG23	1:B:374:GLY:HA2	2.01	0.42
1:A:244:VAL:HG12	1:A:246:LEU:HD12	2.01	0.42
1:B:429:ILE:HD12	1:B:430:ALA:H	1.84	0.42
1:B:187:ASN:O	1:B:189:ILE:HG13	2.20	0.42
1:B:294:GLU:HA	1:B:294:GLU:OE2	2.20	0.42
1:A:303:TRP:CE2	1:A:308:HIS:NE2	2.88	0.42
1:B:285:VAL:HA	1:B:354:GLY:O	2.20	0.42
1:A:244:VAL:HB	1:A:277:MET:CE	2.50	0.42
1:A:11:GLU:HG2	1:A:39:TRP:CZ3	2.55	0.41
1:A:309:LEU:HD12	1:A:341:MET:SD	2.60	0.41
1:B:111:HIS:HA	1:B:112:PRO:HD3	1.76	0.41
1:A:397:LEU:HD12	1:A:397:LEU:HA	1.90	0.41
1:B:226:GLN:NE2	1:B:228:GLY:N	2.59	0.41
1:B:381:VAL:CG1	1:B:384:GLY:HA3	2.49	0.41
1:B:232:ARG:NH1	2:B:538:HOH:O	2.48	0.41
1:B:166:GLU:CG	1:B:170:LYS:HE3	2.48	0.41
1:A:334:VAL:O	1:A:338:ILE:HG13	2.20	0.41
1:A:408:GLU:HG2	2:A:471:HOH:O	2.19	0.41
1:B:14:CYS:HB2	2:B:531:HOH:O	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:171:LEU:HG	1:B:199:ILE:HD13	2.01	0.41
1:A:286:GLY:O	1:A:355:THR:HA	2.20	0.41
1:A:11:GLU:HG3	1:A:12:MET:N	2.36	0.41
1:A:11:GLU:HG2	1:A:39:TRP:HZ3	1.85	0.41
1:A:87:MET:CE	1:B:87:MET:HE2	2.51	0.41
1:B:223:VAL:HA	1:B:413:ARG:NH1	2.36	0.41
1:B:340:ASN:O	1:B:343:LYS:HG2	2.20	0.41
1:B:102:ALA:HA	1:B:131:ALA:HB3	2.02	0.41
1:A:219:GLN:HE22	1:A:412:TYR:HB3	1.86	0.41
1:A:61:GLY:HA2	1:A:141:SER:OG	2.20	0.41
1:A:380:TYR:H	1:A:385:THR:CG2	2.24	0.41
1:A:285:VAL:HG11	1:A:393:VAL:HG22	2.03	0.41
1:A:80:ILE:HA	1:A:81:PRO:C	2.40	0.41
1:B:35:ASP:HA	2:B:580:HOH:O	2.21	0.41
1:B:429:ILE:H	1:B:429:ILE:HG13	1.68	0.40
1:A:55:PHE:HD2	1:A:56:LEU:N	2.20	0.40
1:B:397:LEU:HA	1:B:397:LEU:HD12	1.92	0.40
1:A:66:TYR:O	1:A:67:ARG:HB2	2.22	0.40
1:A:127:LYS:HG2	2:A:525:HOH:O	2.22	0.40
1:A:91:ALA:HA	1:B:91:ALA:HA	2.03	0.40
1:B:154:HIS:CE1	1:B:158:TYR:HE1	2.39	0.40
1:A:150:LYS:CD	1:A:150:LYS:O	2.63	0.40
1:A:27:GLU:HG2	2:A:507:HOH:O	2.20	0.40
1:B:80:ILE:HG13	1:B:81:PRO:HA	2.03	0.40
1:B:86:LEU:HD21	1:B:119:MET:HE1	2.02	0.40
1:A:290:ASP:O	1:A:294:GLU:HG3	2.21	0.40
1:B:358:LYS:O	1:B:362:GLU:HG3	2.22	0.40
1:A:193:PRO:HA	1:B:74:VAL:HG11	2.02	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	431/440 (98%)	403 (94%)	25 (6%)	3 (1%)	30 62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	432/440 (98%)	400 (93%)	29 (7%)	3 (1%)	30	62
All	All	863/880 (98%)	803 (93%)	54 (6%)	6 (1%)	30	62

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	331	SER
1	B	149	LYS
1	A	139	LEU
1	A	329	ILE
1	B	424	LEU
1	B	384	GLY

### 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	372/379 (98%)	352 (95%)	20 (5%)	31	61
1	B	373/379 (98%)	347 (93%)	26 (7%)	21	47
All	All	745/758 (98%)	699 (94%)	46 (6%)	26	54

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	PHE
1	A	13	ASN
1	A	28	ASN
1	A	54	LEU
1	A	55	PHE
1	A	82	VAL
1	A	95	VAL
1	A	135	VAL
1	A	149	LYS
1	A	150	LYS
1	A	155	ASP
1	A	226	GLN

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Mol	Chain	Res	Type
1	A	246	LEU
1	A	249	LYS
1	A	309	LEU
1	A	327	ASP
1	A	366	LEU
1	A	385	THR
1	A	397	LEU
1	A	424	LEU
1	B	3	LYS
1	B	13	ASN
1	B	28	ASN
1	B	48	LYS
1	B	52	ASP
1	B	54	LEU
1	B	55	PHE
1	B	95	VAL
1	B	138	HIS
1	B	153	GLU
1	B	156	GLU
1	B	226	GLN
1	B	232	ARG
1	B	246	LEU
1	B	273	ASP
1	B	285	VAL
1	B	305	LEU
1	B	326	ASN
1	B	332	ILE
1	B	347	LYS
1	B	366	LEU
1	B	380	TYR
1	B	397	LEU
1	B	409	GLU
1	B	424	LEU
1	B	429	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	13	ASN
1	A	20	HIS
1	A	25	HIS

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Mol	Chain	Res	Type
1	A	28	ASN
1	A	29	GLN
1	A	31	HIS
1	A	68	GLN
1	A	83	ASN
1	A	111	HIS
1	A	115	HIS
1	A	138	HIS
1	A	154	HIS
1	A	219	GLN
1	A	226	GLN
1	A	274	HIS
1	A	297	ASN
1	A	339	ASN
1	A	340	ASN
1	A	379	GLN
1	A	398	GLN
1	B	20	HIS
1	B	28	ASN
1	B	29	GLN
1	B	83	ASN
1	B	111	HIS
1	B	179	ASN
1	B	219	GLN
1	B	226	GLN
1	B	274	HIS
1	B	300	GLN
1	B	311	HIS
1	B	379	GLN
1	B	398	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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	433/440 (98%)	-0.34	3 (0%) 84 89	20, 32, 54, 71	0
1	B	434/440 (98%)	-0.29	7 (1%) 68 74	19, 34, 58, 78	0
All	All	867/880 (98%)	-0.31	10 (1%) 75 81	19, 34, 56, 78	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	329	ILE	5.1
1	A	329	ILE	4.1
1	B	331	SER	3.3
1	B	330	GLY	3.2
1	B	328	TYR	2.9
1	B	334	VAL	2.8
1	B	332	ILE	2.6
1	A	328	TYR	2.3
1	B	1	MET	2.0
1	A	323	TYR	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 ⓘ

There are no such residues in this entry.