



# Full wwPDB X-ray Structure Validation Report

Apr 21, 2014 – 11:34 PM EDT

PDB ID : 1YBE  
Title : Crystal Structure of a Nicotinate phosphoribosyltransferase  
Authors : Seetharaman, J.; Swaminathan, S.; Burley, S.K.; New York SGX Research  
Center for Structural Genomics (NYSGXRC)  
Deposited on : 2004-12-20  
Resolution : 2.50 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>

---

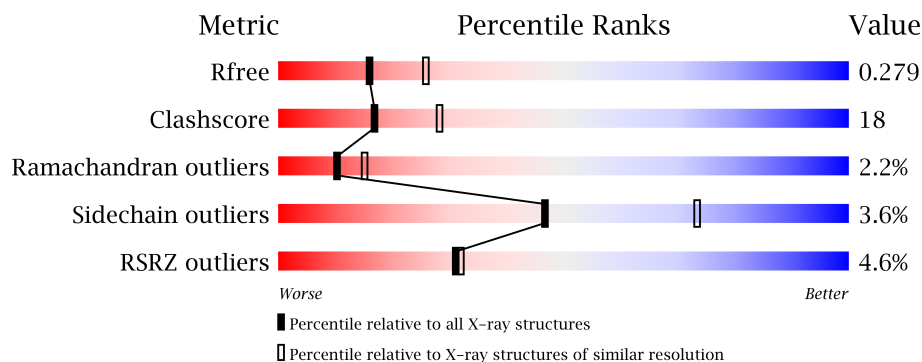
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : stable22978  
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) : stable22978

# 1 Overall quality at a glance

The reported resolution of this entry is 2.50 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	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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	449	
1	B	449	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6910 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 Nicotinate phosphoribosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	416	Total	C	N	O	S	0	0	0
			3293	2104	569	606	14			
1	B	416	Total	C	N	O	S	0	0	0
			3293	2104	569	606	14			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	CLONING ARTIFACT	UNP Q8UIS9
A	2	SER	-	CLONING ARTIFACT	UNP Q8UIS9
A	3	LEU	-	CLONING ARTIFACT	UNP Q8UIS9
A	4	GLY	-	CLONING ARTIFACT	UNP Q8UIS9
A	5	ASN	-	CLONING ARTIFACT	UNP Q8UIS9
A	6	ALA	-	CLONING ARTIFACT	UNP Q8UIS9
A	7	SER	-	CLONING ARTIFACT	UNP Q8UIS9
A	442	GLU	-	EXPRESSION TAG	UNP Q8UIS9
A	443	GLY	-	EXPRESSION TAG	UNP Q8UIS9
A	444	HIS	-	EXPRESSION TAG	UNP Q8UIS9
A	445	HIS	-	EXPRESSION TAG	UNP Q8UIS9
A	446	HIS	-	EXPRESSION TAG	UNP Q8UIS9
A	447	HIS	-	EXPRESSION TAG	UNP Q8UIS9
A	448	HIS	-	EXPRESSION TAG	UNP Q8UIS9
A	449	HIS	-	EXPRESSION TAG	UNP Q8UIS9
B	1	MET	-	CLONING ARTIFACT	UNP Q8UIS9
B	2	SER	-	CLONING ARTIFACT	UNP Q8UIS9
B	3	LEU	-	CLONING ARTIFACT	UNP Q8UIS9
B	4	GLY	-	CLONING ARTIFACT	UNP Q8UIS9
B	5	ASN	-	CLONING ARTIFACT	UNP Q8UIS9
B	6	ALA	-	CLONING ARTIFACT	UNP Q8UIS9
B	7	SER	-	CLONING ARTIFACT	UNP Q8UIS9
B	442	GLU	-	EXPRESSION TAG	UNP Q8UIS9
B	443	GLY	-	EXPRESSION TAG	UNP Q8UIS9
B	444	HIS	-	EXPRESSION TAG	UNP Q8UIS9

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	445	HIS	-	EXPRESSION TAG	UNP Q8UIS9
B	446	HIS	-	EXPRESSION TAG	UNP Q8UIS9
B	447	HIS	-	EXPRESSION TAG	UNP Q8UIS9
B	448	HIS	-	EXPRESSION TAG	UNP Q8UIS9
B	449	HIS	-	EXPRESSION TAG	UNP Q8UIS9

- Molecule 2 is water.

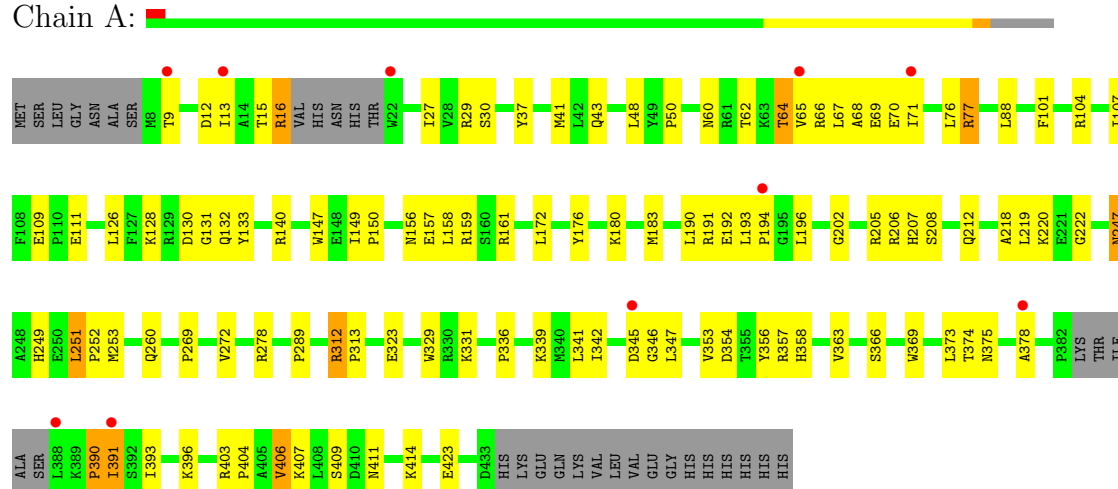
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	230	Total	O	0	0
			230	230		
2	B	94	Total	O	0	0
			94	94		

### 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.

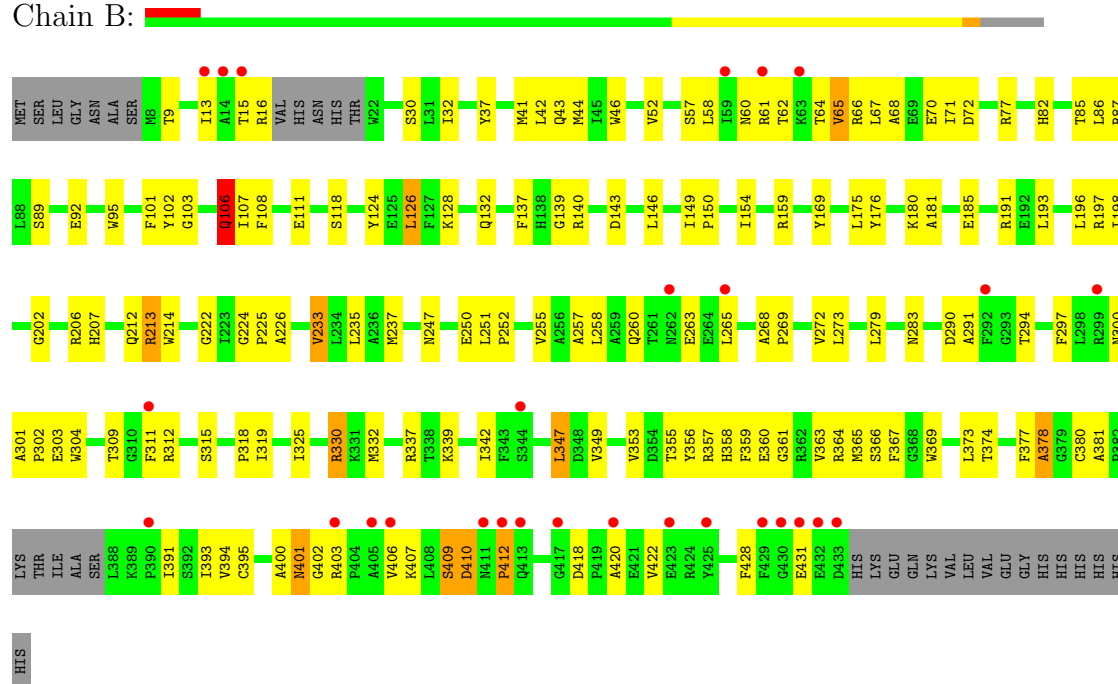
#### • Molecule 1: Nicotinate phosphoribosyltransferase

Chain A:



#### • Molecule 1: Nicotinate phosphoribosyltransferase

Chain B:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	179.77Å 69.43Å 87.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.36 – 2.50 45.36 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.4 (45.36-2.50) 98.1 (45.36-2.50)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.46 (at 2.48Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.222 , 0.272 0.234 , 0.279	Depositor DCC
$R_{free}$ test set	3895 reflections (10.16%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.3	Xtriage
Anisotropy	0.327	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 33.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 38426 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6910	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% of the height of the origin peak. No significant pseudotranslation is detected.*

<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	0.40	0/3372	0.62	0/4578
1	B	0.35	0/3372	0.56	0/4578
All	All	0.38	0/6744	0.59	0/9156

There are no bond length outliers.

There are no bond angle outliers.

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	3293	0	3182	96	0
1	B	3293	0	3181	135	0
2	A	230	0	0	17	0
2	B	94	0	0	9	0
All	All	6910	0	6363	231	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 18.

All (231) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:312:ARG:HG2	1:A:312:ARG:HH11	1.23	1.04

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:198:ILE:HD11	1:B:369:TRP:HB2	1.49	0.95
1:A:68:ALA:HB1	1:A:128:LYS:HE3	1.54	0.87
1:B:68:ALA:HB1	1:B:128:LYS:NZ	1.91	0.86
1:B:87:ARG:HB3	1:B:87:ARG:HH11	1.45	0.82
1:B:66:ARG:HA	1:B:132:GLN:NE2	1.95	0.81
1:B:71:ILE:HD11	1:B:159:ARG:HG2	1.63	0.81
1:A:77:ARG:NE	1:A:126:LEU:HD23	1.97	0.80
1:A:60:ASN:HD22	1:A:132:GLN:HE22	1.30	0.79
1:B:87:ARG:HB3	1:B:87:ARG:NH1	1.96	0.79
1:B:66:ARG:HA	1:B:132:GLN:HE22	1.48	0.78
1:A:104:ARG:HG3	2:A:574:HOH:O	1.82	0.78
1:B:213:ARG:HH11	1:B:213:ARG:HB3	1.47	0.78
1:A:206:ARG:HA	1:A:374:THR:HG23	1.67	0.75
1:B:68:ALA:HB1	1:B:128:LYS:HZ3	1.48	0.75
1:B:193:LEU:O	1:B:196:LEU:HG	1.86	0.75
1:B:101:PHE:O	1:B:103:GLY:N	2.20	0.74
1:B:202:GLY:O	1:B:374:THR:HG21	1.88	0.74
1:B:82:HIS:O	1:B:85:THR:HB	1.87	0.73
1:B:198:ILE:HD12	1:B:367:PHE:O	1.89	0.72
1:A:357:ARG:HH11	1:A:357:ARG:HG3	1.55	0.72
1:B:32:ILE:HB	1:B:233:VAL:CG2	2.19	0.72
1:B:315:SER:HB2	1:B:410:ASP:HB2	1.72	0.71
1:A:312:ARG:HG2	1:A:312:ARG:NH1	2.03	0.71
1:B:44:MET:CE	1:B:251:LEU:HD11	2.21	0.70
1:A:16:ARG:HH11	1:A:16:ARG:HG3	1.56	0.70
1:A:220:LYS:HE3	2:A:494:HOH:O	1.89	0.70
1:A:77:ARG:HE	1:A:126:LEU:HD23	1.54	0.70
1:B:89:SER:OG	1:B:92:GLU:HG3	1.91	0.70
1:B:197:ARG:HH11	1:B:226:ALA:HA	1.58	0.69
1:A:219:LEU:HD21	1:A:369:TRP:HZ3	1.58	0.69
1:A:71:ILE:HD12	1:A:158:LEU:HB3	1.74	0.68
1:B:206:ARG:HH11	1:B:212:GLN:HE22	1.42	0.68
1:B:418:ASP:O	1:B:422:VAL:HG23	1.95	0.67
1:B:258:LEU:CD2	1:B:401:ASN:HD22	2.07	0.67
1:B:16:ARG:HG2	2:B:496:HOH:O	1.93	0.67
1:A:76:LEU:HD23	1:A:126:LEU:HD21	1.77	0.67
1:A:43:GLN:HE22	1:A:109:GLU:H	1.44	0.66
1:A:60:ASN:HD22	1:A:132:GLN:NE2	1.93	0.66
1:B:403:ARG:H	1:B:403:ARG:HD2	1.61	0.66
1:B:364:ARG:HD2	2:B:528:HOH:O	1.94	0.65
1:B:30:SER:HB2	2:B:523:HOH:O	1.96	0.65
1:A:202:GLY:O	1:A:374:THR:HG21	1.96	0.65

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:400:ALA:C	1:B:402:GLY:H	2.00	0.65
1:A:249:HIS:O	1:A:252:PRO:HD2	1.97	0.64
1:A:149:ILE:HB	1:A:150:PRO:HD3	1.79	0.64
1:A:390:PRO:HG2	1:A:391:ILE:H	1.63	0.63
1:B:258:LEU:HD21	1:B:401:ASN:HD22	1.63	0.63
1:B:319:ILE:HG23	1:B:358:HIS:CE1	2.34	0.63
1:A:206:ARG:HH11	1:A:212:GLN:NE2	1.96	0.63
1:A:48:LEU:HD22	1:A:278:ARG:NH2	2.14	0.63
1:A:159:ARG:C	1:A:159:ARG:HD3	2.19	0.62
1:B:265:LEU:HD12	1:B:428:PHE:CE2	2.34	0.61
1:B:337:ARG:HG3	1:B:337:ARG:HH11	1.66	0.61
1:B:268:ALA:N	1:B:269:PRO:HD2	2.16	0.61
1:B:87:ARG:CB	1:B:87:ARG:HH11	2.12	0.61
1:B:265:LEU:HD12	1:B:428:PHE:HE2	1.67	0.60
1:B:58:LEU:HD12	1:B:394:VAL:O	2.01	0.59
1:A:41:MET:SD	1:A:251:LEU:HD12	2.42	0.59
1:B:363:VAL:HG22	1:B:364:ARG:N	2.17	0.59
1:A:70:GLU:O	1:A:71:ILE:HD13	2.03	0.59
1:B:315:SER:OG	1:B:409:SER:HB2	2.03	0.58
1:B:149:ILE:HB	1:B:150:PRO:HD3	1.84	0.58
1:A:251:LEU:CB	1:A:252:PRO:HD3	2.34	0.58
1:A:206:ARG:HH11	1:A:212:GLN:HE22	1.52	0.58
1:B:150:PRO:O	1:B:154:ILE:HG13	2.03	0.57
1:B:412:PRO:HG2	1:B:431:GLU:OE2	2.04	0.57
1:A:156:ASN:OD1	1:A:205:ARG:HA	2.04	0.57
1:B:44:MET:HE2	1:B:251:LEU:HD11	1.86	0.57
1:B:62:THR:HG22	1:B:64:THR:O	2.04	0.57
1:B:41:MET:HE1	1:B:250:GLU:HG2	1.87	0.57
1:A:15:THR:O	1:A:15:THR:HG22	2.04	0.57
1:B:44:MET:HE1	1:B:251:LEU:HD11	1.87	0.57
1:B:62:THR:HG21	1:B:391:ILE:HG22	1.86	0.57
1:A:27:ILE:HD13	1:A:161:ARG:NH2	2.20	0.57
1:A:219:LEU:HD21	1:A:369:TRP:CZ3	2.40	0.57
1:A:12:ASP:O	1:A:16:ARG:HD3	2.05	0.56
1:B:196:LEU:HD12	1:B:226:ALA:HB1	1.86	0.56
1:A:194:PRO:HD2	2:A:458:HOH:O	2.06	0.55
1:B:64:THR:O	1:B:65:VAL:HB	2.04	0.55
1:A:312:ARG:CG	1:A:312:ARG:HH11	2.05	0.54
1:B:32:ILE:O	1:B:233:VAL:HG22	2.07	0.54
1:B:369:TRP:CE3	1:B:373:LEU:HD13	2.43	0.54
1:B:67:LEU:CD2	1:B:159:ARG:HD3	2.37	0.54
1:A:111:GLU:HB2	2:A:485:HOH:O	2.08	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:206:ARG:HA	1:A:374:THR:CG2	2.37	0.54
1:A:43:GLN:NE2	1:A:109:GLU:H	2.05	0.53
1:A:192:GLU:C	1:A:193:LEU:HD12	2.28	0.53
1:B:42:LEU:HD12	1:B:42:LEU:O	2.09	0.53
1:A:396:LYS:NZ	2:A:533:HOH:O	2.42	0.53
1:B:37:TYR:O	1:B:41:MET:HG3	2.09	0.53
1:B:400:ALA:O	1:B:402:GLY:N	2.42	0.53
1:A:357:ARG:NH1	1:A:357:ARG:HG3	2.20	0.52
1:B:357:ARG:NH2	2:B:510:HOH:O	2.42	0.52
1:A:353:VAL:HG23	1:A:354:ASP:N	2.25	0.52
1:A:9:THR:O	1:A:13:ILE:HG12	2.08	0.52
1:B:176:TYR:OH	1:B:207:HIS:HE1	1.93	0.52
1:A:50:PRO:O	1:A:140:ARG:HD2	2.10	0.52
1:A:68:ALA:HB1	1:A:128:LYS:CE	2.34	0.52
1:B:255:VAL:O	1:B:255:VAL:HG12	2.10	0.51
1:B:330:ARG:HH11	1:B:330:ARG:HA	1.75	0.51
1:A:312:ARG:HD2	2:A:610:HOH:O	2.11	0.51
1:A:345:ASP:CG	1:A:346:GLY:H	2.14	0.51
1:B:339:LYS:O	1:B:364:ARG:HB2	2.11	0.51
1:A:176:TYR:OH	1:A:207:HIS:HE1	1.94	0.51
1:A:68:ALA:HA	1:A:133:TYR:CE1	2.46	0.51
1:A:104:ARG:HD3	2:A:575:HOH:O	2.10	0.51
1:B:106:GLN:HA	2:B:465:HOH:O	2.09	0.51
1:B:32:ILE:HB	1:B:233:VAL:HG22	1.93	0.50
1:B:9:THR:O	1:B:13:ILE:HG12	2.11	0.50
1:B:342:ILE:HG12	1:B:366:SER:HB3	1.93	0.50
1:B:290:ASP:O	1:B:291:ALA:C	2.50	0.50
1:B:260:GLN:HE21	1:B:403:ARG:NH2	2.10	0.50
1:A:16:ARG:HG3	1:A:16:ARG:NH1	2.25	0.50
1:A:347:LEU:HB2	2:A:473:HOH:O	2.10	0.50
1:B:279:LEU:N	1:B:279:LEU:HD12	2.27	0.50
1:A:68:ALA:HB3	1:A:131:GLY:HA2	1.93	0.50
1:A:67:LEU:C	1:A:69:GLU:H	2.13	0.50
1:B:206:ARG:HA	1:B:374:THR:HG23	1.93	0.50
1:A:207:HIS:O	1:A:208:SER:HB3	2.12	0.49
1:B:15:THR:O	1:B:15:THR:HG22	2.11	0.49
1:B:400:ALA:C	1:B:402:GLY:N	2.66	0.49
1:A:193:LEU:HD23	1:A:356:TYR:CD2	2.47	0.49
1:B:41:MET:CE	1:B:250:GLU:HG2	2.42	0.49
1:A:30:SER:HB2	2:A:463:HOH:O	2.12	0.49
1:B:175:LEU:HD13	1:B:381:ALA:HA	1.94	0.49
1:B:71:ILE:HD12	1:B:71:ILE:N	2.27	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:260:GLN:HE22	1:A:403:ARG:NH1	2.09	0.49
1:B:363:VAL:HG22	1:B:364:ARG:H	1.77	0.49
1:A:60:ASN:HA	1:A:393:ILE:HD12	1.94	0.49
1:B:257:ALA:O	1:B:403:ARG:HD3	2.13	0.49
1:B:300:ASN:HD22	1:B:300:ASN:N	2.09	0.49
1:A:207:HIS:HD2	2:A:662:HOH:O	1.96	0.48
1:B:349:VAL:O	1:B:353:VAL:HG23	2.13	0.48
1:A:13:ILE:HD11	2:A:609:HOH:O	2.13	0.48
1:B:283:ASN:HD22	1:B:309:THR:HG21	1.77	0.48
1:B:418:ASP:OD2	1:B:420:ALA:HB3	2.14	0.48
1:B:369:TRP:CZ3	1:B:373:LEU:HD13	2.48	0.48
1:B:330:ARG:NH2	2:B:484:HOH:O	2.47	0.47
1:B:193:LEU:HD21	1:B:357:ARG:NH1	2.30	0.47
1:B:294:THR:O	1:B:297:PHE:HB3	2.14	0.47
1:B:206:ARG:HH11	1:B:212:GLN:NE2	2.09	0.47
1:B:315:SER:CB	1:B:410:ASP:HB2	2.42	0.47
1:B:57:SER:O	1:B:395:CYS:HA	2.15	0.47
1:B:191:ARG:HH21	1:B:222:GLY:HA2	1.80	0.47
1:B:391:ILE:HD12	1:B:391:ILE:O	2.15	0.46
1:A:312:ARG:HG3	1:A:342:ILE:HB	1.97	0.46
1:A:312:ARG:CG	1:A:312:ARG:NH1	2.72	0.46
1:B:52:VAL:HG13	1:B:401:ASN:ND2	2.31	0.46
1:B:302:PRO:HB2	1:B:304:TRP:CE2	2.50	0.46
1:A:247:ASN:ND2	2:A:453:HOH:O	2.49	0.46
1:B:180:LYS:HD3	1:B:214:TRP:CZ2	2.51	0.46
1:B:337:ARG:HG3	1:B:337:ARG:NH1	2.31	0.46
1:B:312:ARG:HG2	1:B:342:ILE:O	2.16	0.45
1:A:249:HIS:O	1:A:253:MET:HG3	2.17	0.45
1:B:140:ARG:HB2	1:B:143:ASP:OD1	2.16	0.45
1:B:107:ILE:HG23	2:B:495:HOH:O	2.16	0.45
1:B:355:THR:HG22	1:B:365:MET:CE	2.47	0.45
1:A:104:ARG:HG2	2:A:575:HOH:O	2.16	0.45
1:B:213:ARG:HH11	1:B:213:ARG:CB	2.24	0.45
1:B:30:SER:HA	1:B:86:LEU:HD13	1.99	0.45
1:A:77:ARG:CD	1:A:126:LEU:HD23	2.47	0.45
1:A:60:ASN:ND2	1:A:132:GLN:HE22	2.05	0.45
1:A:62:THR:CG2	1:A:64:THR:HG23	2.46	0.45
1:B:107:ILE:HG13	1:B:108:PHE:CD1	2.51	0.45
1:B:70:GLU:CD	1:B:159:ARG:HH11	2.19	0.45
1:A:269:PRO:O	1:A:272:VAL:HG22	2.16	0.45
1:A:27:ILE:HD12	1:A:157:GLU:CG	2.47	0.44
1:B:235:LEU:HD23	2:B:517:HOH:O	2.17	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:377:PHE:O	1:B:378:ALA:C	2.55	0.44
1:A:249:HIS:C	1:A:252:PRO:HD2	2.37	0.44
1:B:60:ASN:C	1:B:62:THR:H	2.20	0.44
1:B:77:ARG:HG2	1:B:126:LEU:HD12	2.00	0.44
1:A:176:TYR:O	1:A:180:LYS:HG3	2.18	0.44
1:B:106:GLN:HB3	1:B:106:GLN:HE21	1.55	0.44
1:B:224:GLY:HA3	1:B:225:PRO:HD3	1.82	0.44
1:B:356:TYR:HA	1:B:365:MET:HE1	1.99	0.44
1:A:411:ASN:HD22	1:A:414:LYS:HD2	1.81	0.44
1:B:68:ALA:HB1	1:B:128:LYS:HZ1	1.75	0.44
1:A:251:LEU:HB2	1:A:252:PRO:HD3	2.00	0.44
1:A:342:ILE:HG12	1:A:366:SER:HB3	2.00	0.44
1:B:369:TRP:CD2	1:B:373:LEU:HB2	2.53	0.44
1:A:313:PRO:HA	2:A:520:HOH:O	2.17	0.43
1:B:251:LEU:HB3	1:B:252:PRO:CD	2.48	0.43
1:A:423:GLU:HG2	2:A:643:HOH:O	2.17	0.43
1:B:58:LEU:HG	1:B:393:ILE:HD11	2.00	0.43
1:B:87:ARG:NH2	1:B:118:SER:HA	2.33	0.43
1:A:329:TRP:CZ2	1:A:339:LYS:HG2	2.53	0.43
1:A:341:LEU:HD12	1:A:363:VAL:HG11	1.99	0.43
1:B:181:ALA:O	1:B:185:GLU:HG3	2.19	0.43
1:A:353:VAL:CG2	1:A:354:ASP:N	2.82	0.43
1:B:251:LEU:HB3	1:B:252:PRO:HD3	2.00	0.43
1:A:406:VAL:HG13	1:A:407:LYS:N	2.34	0.43
1:A:323:GLU:OE2	1:A:358:HIS:HE1	2.02	0.43
1:A:403:ARG:HA	1:A:404:PRO:HD3	1.84	0.43
1:B:347:LEU:HD12	1:B:347:LEU:H	1.83	0.43
1:A:130:ASP:N	1:A:130:ASP:OD2	2.52	0.42
1:B:46:TRP:HH2	1:B:111:GLU:HB3	1.84	0.42
1:B:32:ILE:HB	1:B:233:VAL:HG21	1.96	0.42
1:B:260:GLN:NE2	1:B:403:ARG:NH2	2.67	0.42
1:B:175:LEU:HA	1:B:380:CYS:O	2.19	0.42
1:A:191:ARG:NE	1:A:222:GLY:O	2.53	0.42
1:A:336:PRO:O	1:A:363:VAL:HG23	2.19	0.42
1:B:67:LEU:HD23	1:B:70:GLU:OE1	2.20	0.42
1:A:27:ILE:HD12	1:A:157:GLU:HG2	2.01	0.41
1:B:359:PHE:O	1:B:360:GLU:C	2.59	0.41
1:B:315:SER:CB	1:B:410:ASP:H	2.32	0.41
1:A:101:PHE:HB2	1:A:107:ILE:HD13	2.02	0.41
1:A:132:GLN:NE2	2:A:582:HOH:O	2.53	0.41
1:B:44:MET:HA	1:B:279:LEU:CD2	2.50	0.41
1:B:43:GLN:HE22	1:B:108:PHE:HA	1.86	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:124:TYR:HB3	1:B:137:PHE:CE2	2.55	0.41
1:B:107:ILE:HD11	1:B:108:PHE:CE1	2.55	0.41
1:B:42:LEU:HD22	1:B:146:LEU:HG	2.03	0.41
1:B:70:GLU:OE2	1:B:159:ARG:NH1	2.53	0.41
1:B:406:VAL:CG1	1:B:407:LYS:N	2.84	0.41
1:A:159:ARG:O	1:A:159:ARG:HD3	2.21	0.41
1:B:139:GLY:HA3	2:B:533:HOH:O	2.21	0.41
1:B:363:VAL:CG2	1:B:364:ARG:N	2.83	0.41
1:A:37:TYR:CD1	1:A:41:MET:HE2	2.56	0.41
1:B:272:VAL:HG23	1:B:273:LEU:N	2.36	0.41
1:A:331:LYS:HE2	1:A:331:LYS:HB2	1.84	0.41
1:A:369:TRP:CZ3	1:A:373:LEU:HD13	2.56	0.41
1:B:311:PHE:HB3	1:B:325:ILE:HD13	2.02	0.41
1:A:190:LEU:HD22	1:A:196:LEU:HD21	2.02	0.40
1:B:58:LEU:CG	1:B:393:ILE:HD11	2.51	0.40
1:B:95:TRP:CD2	1:B:237:MET:HG3	2.56	0.40
1:B:140:ARG:HH11	1:B:140:ARG:HG3	1.87	0.40
1:B:52:VAL:HG11	1:B:258:LEU:HD11	2.02	0.40
1:A:183:MET:HE2	1:A:218:ALA:CB	2.52	0.40
1:A:29:ARG:NH1	2:A:653:HOH: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	410/449 (91%)	374 (91%)	30 (7%)	6 (2%)	15	25
1	B	410/449 (91%)	366 (89%)	32 (8%)	12 (3%)	7	9
All	All	820/898 (91%)	740 (90%)	62 (8%)	18 (2%)	10	15

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	66	ARG
1	A	390	PRO
1	B	102	TYR
1	B	169	TYR
1	B	378	ALA
1	A	409	SER
1	B	361	GLY
1	B	409	SER
1	B	61	ARG
1	B	301	ALA
1	B	401	ASN
1	A	378	ALA
1	A	65	VAL
1	A	391	ILE
1	B	65	VAL
1	B	106	GLN
1	B	412	PRO
1	B	318	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	336/385 (87%)	324 (96%)	12 (4%)	47	73
1	B	336/385 (87%)	324 (96%)	12 (4%)	47	73
All	All	672/770 (87%)	648 (96%)	24 (4%)	47	73

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ARG
1	A	64	THR
1	A	77	ARG
1	A	88	LEU
1	A	147	TRP
1	A	172	LEU
1	A	247	ASN
1	A	251	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	289	PRO
1	A	312	ARG
1	A	375	ASN
1	A	406	VAL
1	B	72	ASP
1	B	106	GLN
1	B	126	LEU
1	B	213	ARG
1	B	233	VAL
1	B	247	ASN
1	B	263	GLU
1	B	303	GLU
1	B	330	ARG
1	B	332	MET
1	B	347	LEU
1	B	410	ASP

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

Mol	Chain	Res	Type
1	A	43	GLN
1	A	60	ASN
1	A	106	GLN
1	A	120	GLN
1	A	132	GLN
1	A	207	HIS
1	A	212	GLN
1	A	247	ASN
1	A	262	ASN
1	A	283	ASN
1	A	358	HIS
1	A	375	ASN
1	A	411	ASN
1	B	43	GLN
1	B	106	GLN
1	B	207	HIS
1	B	212	GLN
1	B	247	ASN
1	B	260	GLN
1	B	283	ASN
1	B	300	ASN
1	B	358	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	401	ASN

### 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	416/449 (92%)	0.01	10 (2%) 56 58	14, 30, 59, 74	0
1	B	416/449 (92%)	0.41	28 (6%) 17 17	17, 48, 73, 82	0
All	All	832/898 (92%)	0.21	38 (4%) 31 32	14, 39, 69, 82	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	433	ASP	5.0
1	A	65	VAL	4.5
1	A	22	TRP	4.1
1	B	425	TYR	4.1
1	B	413	GLN	4.0
1	B	432	GLU	4.0
1	B	412	PRO	3.9
1	A	388	LEU	3.4
1	B	13	ILE	3.4
1	B	403	ARG	3.3
1	B	61	ARG	3.1
1	B	429	PHE	3.1
1	A	13	ILE	2.9
1	B	390	PRO	2.7
1	B	431	GLU	2.7
1	B	292	PHE	2.6
1	A	345	ASP	2.5
1	B	59	ILE	2.5
1	B	14	ALA	2.5
1	A	378	ALA	2.5
1	B	15	THR	2.4
1	A	9	THR	2.4
1	B	311	PHE	2.4
1	A	194	PRO	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	417	GLY	2.3
1	B	344	SER	2.3
1	B	299	ARG	2.3
1	B	423	GLU	2.3
1	B	411	ASN	2.2
1	B	262	ASN	2.2
1	B	405	ALA	2.2
1	B	430	GLY	2.1
1	A	391	ILE	2.1
1	B	420	ALA	2.1
1	B	63	LYS	2.1
1	B	406	VAL	2.0
1	B	265	LEU	2.0
1	A	71	ILE	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.