



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2018 – 03:18 am GMT

PDB ID : 1YBE
Title : Crystal Structure of a Nicotinate phosphoribosyltransferase
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Deposited on : 2004-12-20
Resolution : 2.50 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	trunk30967
Percentile statistics	:	(not set)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk30967

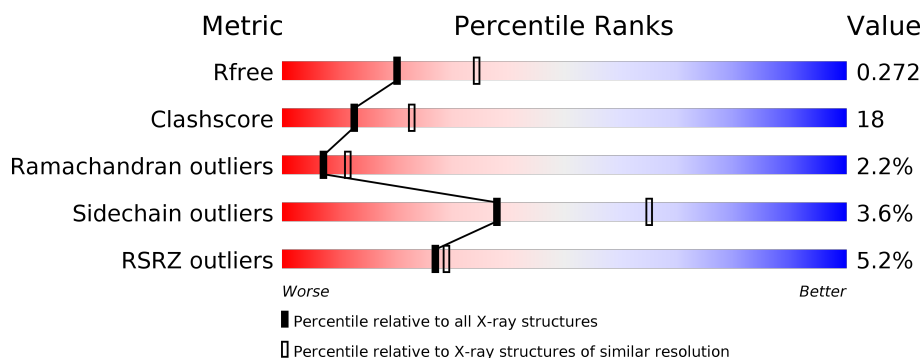
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	111664	4155 (2.50-2.50)
Clashscore	122126	4827 (2.50-2.50)
Ramachandran outliers	120053	4735 (2.50-2.50)
Sidechain outliers	120020	4737 (2.50-2.50)
RSRZ outliers	108989	4058 (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 ≥ 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	449	<div> <div>3%</div> <div> <div></div> <div>68%</div> <div>23%</div> <div>• 7%</div> </div> </div>
1	B	449	<div> <div>7%</div> <div> <div></div> <div>58%</div> <div>32%</div> <div>• 7%</div> </div> </div>

2 Entry composition

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

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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

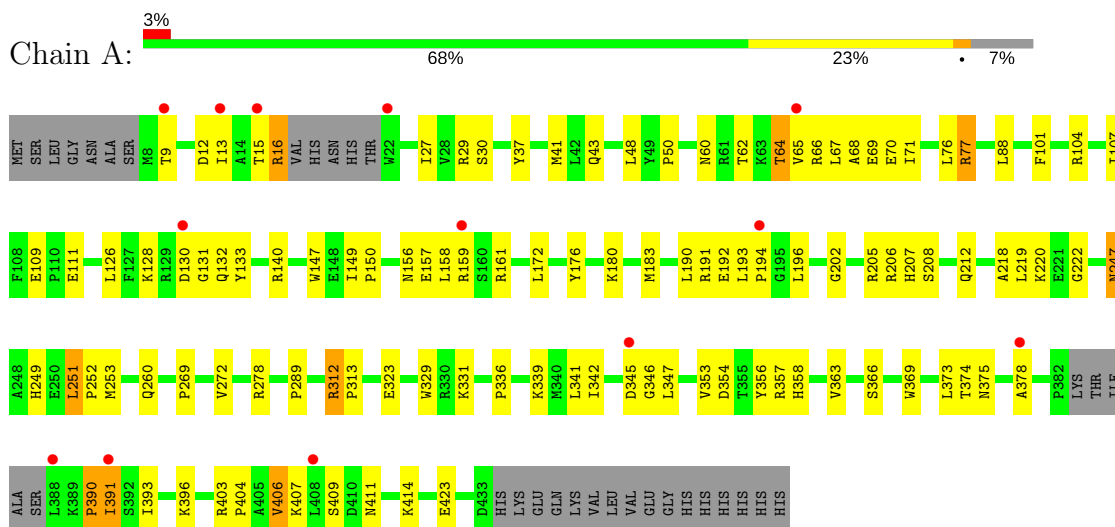
- Molecule 2 is water.

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

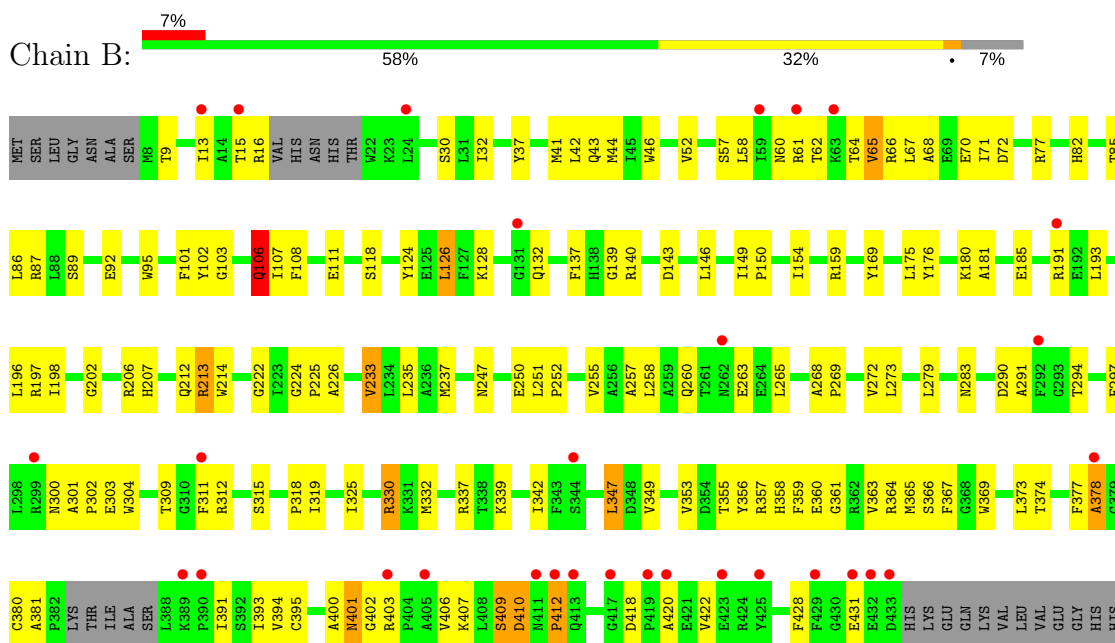
3 Residue-property plots

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



• Molecule 1: Nicotinate phosphoribosyltransferase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 2.48Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.222 , 0.272 0.222 , 0.272	Depositor DCC
R_{free} test set	3895 reflections (10.14%)	wwPDB-VP
Wilson B-factor (Å ²)	36.3	Xtriage
Anisotropy	0.327	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 56.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6910	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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

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 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	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

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 18.

All (231) 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:312:ARG:HG2	1:A:312:ARG:HH11	1.23	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:GLY:O	1:A:374:THR:HG21	1.96	0.65
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:260:GLN:HE21	1:B:403:ARG:NH2	2.10	0.50
1:B:290:ASP:O	1:B:291:ALA:C	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:87:ARG:NH2	1:B:118:SER:HA	2.33	0.43
1:B:58:LEU:HG	1:B:393:ILE:HD11	2.00	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:315:SER:CB	1:B:410:ASP:H	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:359:PHE:O	1:B:360:GLU:C	2.59	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
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%)	11 20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	410/449 (91%)	366 (89%)	32 (8%)	12 (3%)	5	7
All	All	820/898 (91%)	740 (90%)	62 (8%)	18 (2%)	7	11

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%)	38	65
1	B	336/385 (87%)	324 (96%)	12 (4%)	38	65
All	All	672/770 (87%)	648 (96%)	24 (4%)	38	65

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
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

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Mol	Chain	Res	Type
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
1	B	401	ASN

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 carbohydrates 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	416/449 (92%)	-0.02	13 (3%) 49 52	14, 30, 59, 74	0
1	B	416/449 (92%)	0.40	30 (7%) 15 16	17, 48, 73, 82	0
All	All	832/898 (92%)	0.19	43 (5%) 27 29	14, 39, 69, 82	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	433	ASP	5.8
1	A	65	VAL	4.9
1	B	413	GLN	4.7
1	B	432	GLU	4.2
1	A	388	LEU	3.9
1	B	61	ARG	3.9
1	B	425	TYR	3.7
1	B	412	PRO	3.6
1	A	22	TRP	3.5
1	B	390	PRO	3.1
1	A	378	ALA	3.1
1	B	403	ARG	2.9
1	A	391	ILE	2.9
1	B	262	ASN	2.9
1	B	59	ILE	2.8
1	B	429	PHE	2.7
1	B	299	ARG	2.7
1	B	431	GLU	2.7
1	B	423	GLU	2.6
1	B	131	GLY	2.6
1	B	420	ALA	2.6
1	B	15	THR	2.5
1	B	411	ASN	2.5
1	A	345	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	9	THR	2.5
1	B	13	ILE	2.4
1	A	194	PRO	2.4
1	B	389	LYS	2.4
1	A	408	LEU	2.3
1	B	63	LYS	2.2
1	B	417	GLY	2.2
1	B	344	SER	2.2
1	A	159	ARG	2.2
1	A	130	ASP	2.1
1	B	191	ARG	2.1
1	B	405	ALA	2.1
1	B	419	PRO	2.1
1	B	378	ALA	2.1
1	A	15	THR	2.1
1	A	13	ILE	2.1
1	B	24	LEU	2.1
1	B	292	PHE	2.1
1	B	311	PHE	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.