



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 06:44 PM UTC

PDB ID : 2G95 / pdb_00002g95
Title : Crystal Structure of Visfatin/Pre-B Cell Colony Enhancing Factor 1/Nicotinamide Phosphoribosyltransferase
Authors : Kim, M.-K.; Eom, S.H.
Deposited on : 2006-03-05
Resolution : 1.90 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

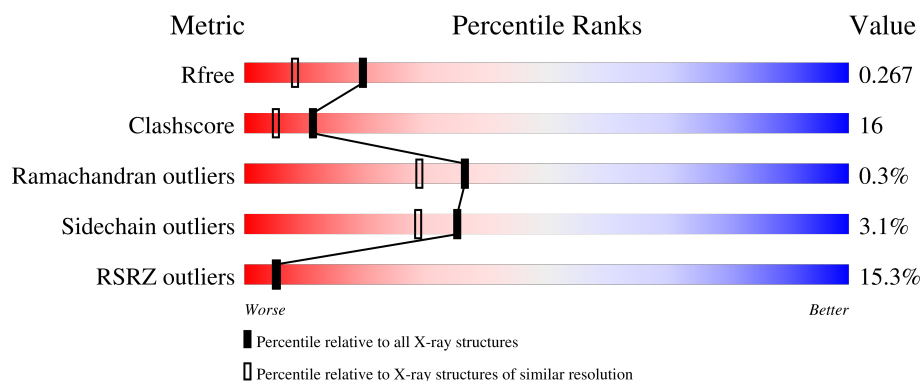
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	491	16% 63% 28% 7%
1	B	491	13% 66% 26% 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7577 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 Nicotinamide phosphoribosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	456	Total	C	N	O	S	0	0	0
			3644	2339	605	694	6			
1	B	460	Total	C	N	O	S	0	0	0
			3682	2360	614	701	7			

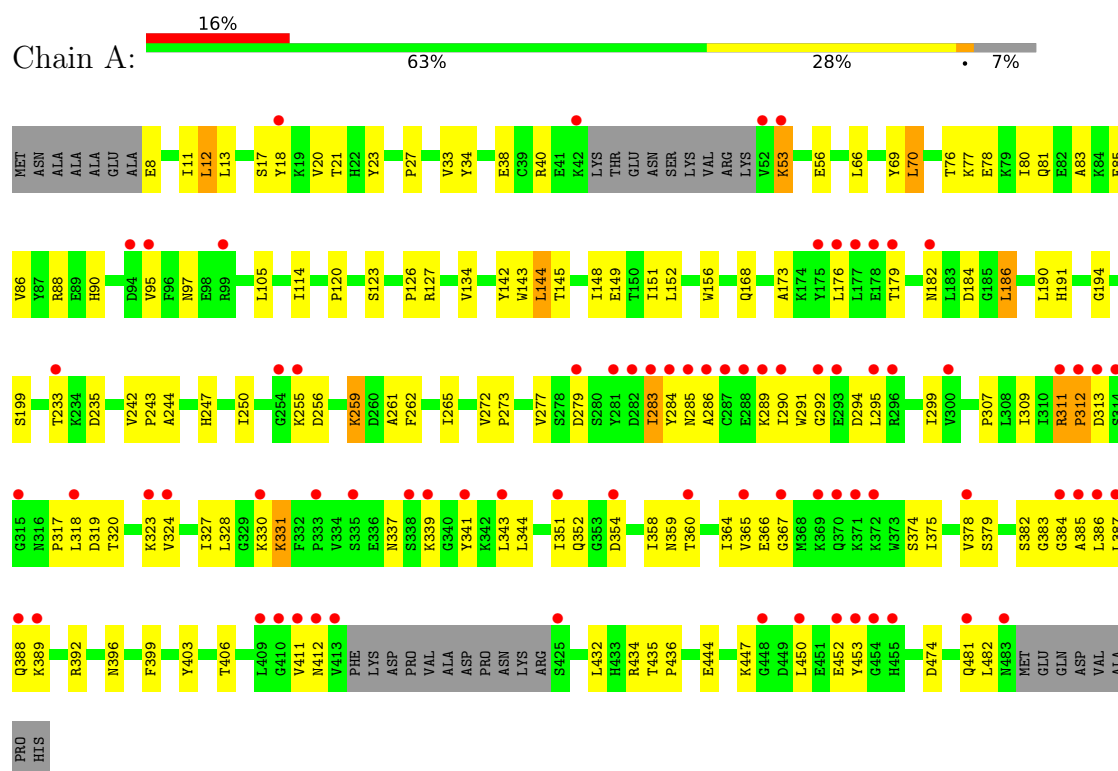
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	104	Total	O	0	0
			104	104		
2	B	147	Total	O	0	0
			147	147		

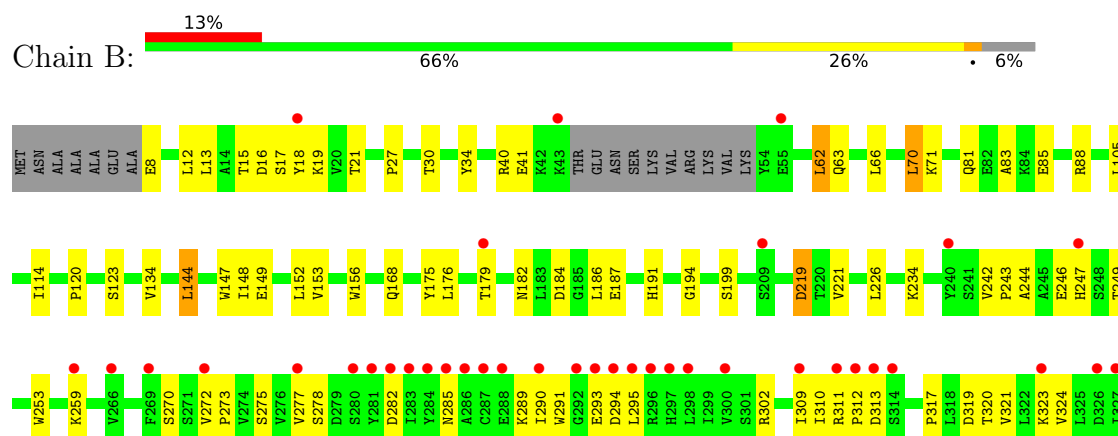
3 Residue-property plots [i](#)

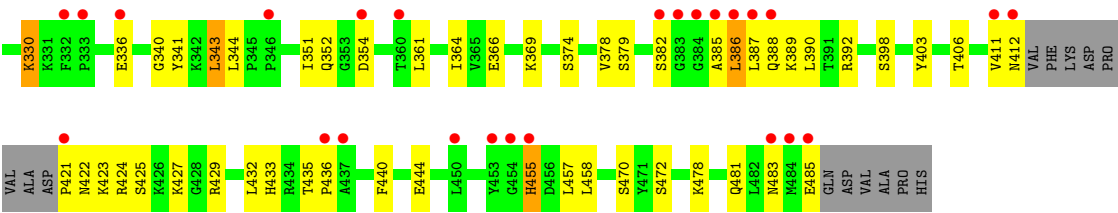
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Nicotinamide phosphoribosyltransferase



- Molecule 1: Nicotinamide phosphoribosyltransferase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.30Å 94.92Å 84.87Å 90.00° 104.91° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 20.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-1.90) 95.2 (20.00-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.04 (at 1.89Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.235 , 0.267 0.235 , 0.267	Depositor DCC
R_{free} test set	8013 reflections (10.02%)	wwPDB-VP
Wilson B-factor (Å ²)	23.0	Xtriage
Anisotropy	0.525	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 40.2	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	0.93	EDS
Total number of atoms	7577	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% 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	0.38	0/3728	0.84	5/5051 (0.1%)
1	B	0.40	0/3767	0.88	10/5100 (0.2%)
All	All	0.39	0/7495	0.86	15/10151 (0.1%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	70	LEU	N-CA-C	7.17	123.15	113.97
1	B	199	SER	N-CA-C	6.47	120.44	112.54
1	A	69	TYR	N-CA-C	6.02	121.50	114.04
1	B	70	LEU	N-CA-C	5.94	120.66	113.41
1	B	378	VAL	N-CA-C	5.75	117.03	108.46
1	B	311	ARG	CA-C-N	5.70	126.50	120.11
1	B	311	ARG	C-N-CA	5.70	126.50	120.11
1	A	199	SER	N-CA-C	5.68	120.06	113.18
1	B	71	LYS	N-CA-C	5.61	118.41	110.50
1	B	30	THR	N-CA-C	-5.39	100.38	108.96
1	B	234	LYS	N-CA-C	-5.23	106.75	113.23
1	A	311	ARG	CA-C-N	5.18	126.31	119.84
1	A	311	ARG	C-N-CA	5.18	126.31	119.84
1	B	17	SER	N-CA-C	5.15	117.29	111.11
1	B	472	SER	N-CA-C	-5.03	103.76	110.55

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3644	0	3615	137	0
1	B	3682	0	3652	108	0
2	A	104	0	0	1	0
2	B	147	0	0	1	0
All	All	7577	0	7267	237	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 16.

All (237) 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:179:THR:HG21	1:A:374:SER:HA	1.27	1.08
1:B:179:THR:HG21	1:B:374:SER:HA	1.39	1.00
1:A:233:THR:HG22	1:A:235:ASP:H	1.28	0.97
1:B:179:THR:CG2	1:B:374:SER:HA	1.98	0.94
1:A:312:PRO:HB2	1:A:320:THR:HG22	1.54	0.88
1:A:179:THR:CG2	1:A:374:SER:HA	2.04	0.87
1:B:385:ALA:HA	1:B:389:LYS:HG3	1.59	0.85
1:B:312:PRO:HB2	1:B:320:THR:HG22	1.61	0.82
1:B:182:ASN:HD22	1:B:184:ASP:H	1.25	0.81
1:B:432:LEU:HD22	1:B:457:LEU:HD12	1.63	0.80
1:A:259:LYS:HG3	1:A:295:LEU:HD11	1.63	0.79
1:B:312:PRO:HB3	1:B:324:VAL:HG21	1.64	0.78
1:A:351:ILE:HG12	1:A:379:SER:OG	1.84	0.77
1:B:432:LEU:HD23	1:B:433:HIS:N	2.00	0.76
1:B:432:LEU:HD21	1:B:440:PHE:HD2	1.50	0.76
1:A:247:HIS:CE1	1:A:277:VAL:HG11	2.22	0.75
1:B:168:GLN:HE22	1:B:386:LEU:HD11	1.52	0.75
1:B:168:GLN:NE2	1:B:386:LEU:HD11	2.02	0.74
1:B:15:THR:HG1	1:B:147:TRP:CD1	2.05	0.74
1:B:312:PRO:HB2	1:B:320:THR:CG2	2.18	0.71
1:A:312:PRO:HB2	1:A:320:THR:CG2	2.20	0.71
1:B:247:HIS:CE1	1:B:277:VAL:HG11	2.26	0.71
1:A:382:SER:HB2	1:A:386:LEU:HG	1.73	0.70
1:A:114:ILE:HG23	1:A:144:LEU:HD13	1.74	0.70
1:A:81:GLN:O	1:A:85:GLU:HG3	1.91	0.69
1:A:168:GLN:HE22	1:A:386:LEU:HD13	1.57	0.69
1:A:182:ASN:HD22	1:A:184:ASP:H	1.40	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:ASN:ND2	1:A:289:LYS:HD2	2.08	0.68
1:A:168:GLN:HE22	1:A:386:LEU:CD1	2.07	0.68
1:A:27:PRO:HB2	1:A:406:THR:HG21	1.75	0.68
1:A:33:VAL:HG11	1:A:142:TYR:O	1.95	0.67
1:B:320:THR:O	1:B:324:VAL:HG23	1.95	0.67
1:A:312:PRO:HB3	1:A:324:VAL:HG21	1.77	0.67
1:B:351:ILE:HG12	1:B:379:SER:OG	1.95	0.67
1:B:424:ARG:HD2	1:B:425:SER:O	1.94	0.66
1:A:283:ILE:HD13	1:A:283:ILE:H	1.61	0.66
1:A:86:VAL:HG11	1:B:221:VAL:HG11	1.78	0.66
1:B:317:PRO:HB2	1:B:364:ILE:HD11	1.77	0.66
1:B:289:LYS:HD2	1:B:289:LYS:N	2.11	0.65
1:B:179:THR:HG23	1:B:341:TYR:CG	2.31	0.65
1:A:233:THR:HG22	1:A:235:ASP:N	2.08	0.65
1:A:179:THR:HG23	1:A:341:TYR:CG	2.33	0.64
1:A:114:ILE:HD13	1:A:148:ILE:HD13	1.79	0.64
1:A:435:THR:HB	1:A:436:PRO:HD2	1.80	0.63
1:B:330:LYS:HB2	1:B:330:LYS:NZ	2.14	0.63
1:B:16:ASP:HB2	1:B:19:LYS:HD2	1.80	0.63
1:A:309:ILE:HG21	1:A:351:ILE:HG13	1.82	0.62
1:B:312:PRO:HD2	1:B:351:ILE:O	2.00	0.62
1:B:105:LEU:C	1:B:105:LEU:HD23	2.25	0.62
1:A:244:ALA:HB3	1:B:18:TYR:HB2	1.82	0.61
1:A:283:ILE:HD13	1:A:283:ILE:N	2.15	0.61
1:B:272:VAL:HG13	1:B:273:PRO:HD2	1.81	0.61
1:B:242:VAL:HG11	1:B:273:PRO:HG2	1.81	0.61
1:B:13:LEU:HD21	1:B:83:ALA:HA	1.83	0.61
1:B:309:ILE:CG2	1:B:351:ILE:HG13	2.31	0.60
1:B:352:GLN:HE21	1:B:354:ASP:H	1.49	0.60
1:B:259:LYS:HG2	1:B:290:ILE:HG12	1.83	0.60
1:A:318:LEU:HG	1:A:364:ILE:HA	1.84	0.59
1:B:66:LEU:HD23	1:B:70:LEU:HD12	1.84	0.59
1:A:337:ASN:HD21	1:A:339:LYS:HB2	1.68	0.59
1:A:13:LEU:HD21	1:A:83:ALA:HA	1.84	0.59
1:A:294:ASP:C	1:A:295:LEU:HD12	2.29	0.58
1:A:18:TYR:HB2	1:B:244:ALA:HB3	1.84	0.58
1:B:176:LEU:HD22	1:B:182:ASN:O	2.03	0.58
1:A:365:VAL:HG13	1:A:375:ILE:CD1	2.33	0.58
1:B:191:HIS:HE1	1:B:219:ASP:OD1	1.87	0.57
1:A:33:VAL:HG13	1:A:145:THR:OG1	2.05	0.57
1:A:194:GLY:HA3	1:A:387:LEU:HD12	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:ARG:O	1:B:88:ARG:HD3	2.04	0.57
1:A:273:PRO:HB3	1:A:307:PRO:HD2	1.85	0.57
1:A:318:LEU:HD11	1:A:367:GLY:HA3	1.86	0.56
1:B:27:PRO:HB2	1:B:406:THR:HG21	1.87	0.56
1:B:313:ASP:O	1:B:320:THR:HG21	2.05	0.56
1:A:444:GLU:O	1:A:447:LYS:HG2	2.06	0.56
1:B:70:LEU:HD11	1:B:152:LEU:HD21	1.87	0.56
1:B:120:PRO:HG2	1:B:123:SER:HB3	1.88	0.56
1:A:176:LEU:HD22	1:A:182:ASN:O	2.07	0.55
1:A:242:VAL:CG1	1:A:273:PRO:HG2	2.37	0.55
1:A:434:ARG:HH11	1:A:434:ARG:HB2	1.72	0.54
1:B:275:SER:HA	1:B:309:ILE:HB	1.88	0.54
1:B:458:LEU:HD12	2:B:627:HOH:O	2.08	0.54
1:A:309:ILE:CG2	1:A:351:ILE:HG13	2.36	0.54
1:A:33:VAL:CG1	1:A:142:TYR:O	2.55	0.54
1:B:317:PRO:O	1:B:321:VAL:HG23	2.07	0.54
1:A:33:VAL:HG13	1:A:145:THR:CB	2.38	0.54
1:B:168:GLN:HE22	1:B:386:LEU:HD21	1.71	0.54
1:B:294:ASP:C	1:B:295:LEU:HD12	2.33	0.54
1:B:382:SER:HB3	1:B:386:LEU:HD23	1.91	0.53
1:B:81:GLN:O	1:B:85:GLU:HG3	2.08	0.53
1:B:134:VAL:HG11	1:B:148:ILE:HD11	1.90	0.53
1:B:272:VAL:CG1	1:B:273:PRO:HD2	2.38	0.53
1:B:114:ILE:HD13	1:B:148:ILE:HD13	1.91	0.53
1:A:53:LYS:HD2	1:A:53:LYS:N	2.23	0.53
1:A:382:SER:CB	1:A:386:LEU:HG	2.37	0.53
1:B:88:ARG:HD3	1:B:88:ARG:C	2.33	0.53
1:A:40:ARG:HD2	2:A:588:HOH:O	2.09	0.53
1:A:291:TRP:CE3	1:A:299:ILE:HD11	2.45	0.52
1:B:319:ASP:O	1:B:323:LYS:HG3	2.08	0.52
1:A:134:VAL:HG11	1:A:148:ILE:HD11	1.91	0.52
1:A:365:VAL:HG13	1:A:375:ILE:HD11	1.90	0.52
1:A:279:ASP:HB2	1:A:313:ASP:HA	1.91	0.52
1:B:34:TYR:HB3	1:B:403:TYR:HB3	1.92	0.52
1:A:114:ILE:CG2	1:A:144:LEU:HD13	2.39	0.52
1:B:282:ASP:CB	1:B:285:ASN:HB3	2.40	0.52
1:A:149:GLU:HG3	1:A:399:PHE:CD2	2.45	0.51
1:B:282:ASP:HB3	1:B:285:ASN:HB3	1.92	0.51
1:A:259:LYS:CG	1:A:295:LEU:HD11	2.36	0.51
1:A:309:ILE:HG21	1:A:351:ILE:CG1	2.40	0.51
1:B:242:VAL:CG1	1:B:273:PRO:HG2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:VAL:HG12	1:A:279:ASP:H	1.74	0.51
1:A:313:ASP:O	1:A:320:THR:HG21	2.10	0.51
1:A:388:GLN:HG3	1:A:389:LYS:H	1.76	0.51
1:A:343:LEU:HD23	1:A:344:LEU:O	2.11	0.51
1:A:27:PRO:HG3	1:B:253:TRP:CG	2.45	0.51
1:B:156:TRP:CG	1:B:392:ARG:HG2	2.46	0.50
1:A:190:LEU:HD23	1:A:191:HIS:N	2.26	0.50
1:B:149:GLU:O	1:B:153:VAL:HG22	2.11	0.50
1:B:270:SER:HA	1:B:302:ARG:HH12	1.76	0.50
1:A:95:VAL:HG12	1:A:95:VAL:O	2.12	0.49
1:B:175:TYR:CE2	1:B:369:LYS:HE3	2.47	0.49
1:A:120:PRO:HG2	1:A:123:SER:OG	2.12	0.49
1:A:261:ALA:O	1:A:265:ILE:HG13	2.12	0.49
1:B:435:THR:HB	1:B:436:PRO:HD2	1.93	0.49
1:A:317:PRO:HB2	1:A:364:ILE:HD11	1.94	0.49
1:B:478:LYS:O	1:B:481:GLN:HG2	2.12	0.49
1:A:17:SER:OG	1:A:90:HIS:HE1	1.95	0.49
1:A:295:LEU:HD12	1:A:295:LEU:N	2.28	0.49
1:B:194:GLY:HA3	1:B:387:LEU:HD12	1.94	0.49
1:A:243:PRO:HB3	1:B:21:THR:HG21	1.95	0.49
1:A:33:VAL:CG1	1:A:145:THR:HB	2.43	0.48
1:A:292:GLY:HA2	1:A:331:LYS:HG2	1.95	0.48
1:A:21:THR:HG22	1:A:95:VAL:CG1	2.43	0.48
1:A:38:GLU:OE1	1:A:40:ARG:HG2	2.13	0.48
1:A:352:GLN:HE21	1:A:354:ASP:H	1.61	0.48
1:B:246:GLU:O	1:B:249:THR:HG22	2.13	0.48
1:A:283:ILE:H	1:A:283:ILE:CD1	2.24	0.48
1:B:114:ILE:HG23	1:B:144:LEU:HD13	1.96	0.48
1:A:309:ILE:N	1:A:309:ILE:HD12	2.28	0.48
1:A:168:GLN:HE22	1:A:386:LEU:CD2	2.27	0.48
1:A:168:GLN:NE2	1:A:386:LEU:HD13	2.26	0.48
1:B:432:LEU:HD21	1:B:440:PHE:CD2	2.40	0.48
1:A:360:THR:O	1:A:364:ILE:HG13	2.13	0.47
1:A:21:THR:HG21	1:B:243:PRO:HB3	1.96	0.47
1:A:351:ILE:HG12	1:A:379:SER:HG	1.79	0.47
1:B:312:PRO:CB	1:B:324:VAL:HG21	2.41	0.47
1:A:156:TRP:CG	1:A:392:ARG:HG2	2.50	0.47
1:A:179:THR:HG21	1:A:374:SER:CA	2.20	0.47
1:A:242:VAL:HG11	1:A:273:PRO:HG2	1.96	0.47
1:A:76:THR:O	1:A:80:ILE:HG13	2.15	0.47
1:B:411:VAL:HG12	1:B:412:ASN:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:LEU:HD22	1:B:344:LEU:O	2.15	0.47
1:A:250:ILE:HD13	1:A:262:PHE:HE1	1.80	0.47
1:B:63:GLN:HE22	1:B:470:SER:CB	2.28	0.47
1:B:388:GLN:C	1:B:390:LEU:H	2.23	0.46
1:A:34:TYR:HB3	1:A:403:TYR:HB3	1.98	0.46
1:B:421:PRO:HG2	1:B:422:ASN:H	1.79	0.46
1:B:455:HIS:ND1	1:B:455:HIS:N	2.63	0.46
1:A:18:TYR:HD2	1:B:219:ASP:OD2	1.99	0.46
1:A:168:GLN:HE22	1:A:386:LEU:HD22	1.80	0.46
1:B:15:THR:OG1	1:B:147:TRP:CD1	2.68	0.46
1:A:312:PRO:HD2	1:A:351:ILE:O	2.16	0.45
1:A:38:GLU:CD	1:A:40:ARG:HG2	2.42	0.45
1:B:429:ARG:HH11	1:B:429:ARG:HG3	1.81	0.45
1:A:33:VAL:HG13	1:A:145:THR:HB	1.99	0.45
1:A:286:ALA:HA	1:A:290:ILE:HD12	1.99	0.45
1:A:17:SER:OG	1:A:90:HIS:CE1	2.69	0.45
1:A:307:PRO:HG2	1:A:309:ILE:HD11	1.98	0.45
1:A:66:LEU:HD23	1:A:70:LEU:HD12	1.99	0.45
1:A:389:LYS:O	1:A:389:LYS:HG2	2.17	0.45
1:B:285:ASN:HA	1:B:289:LYS:HD3	1.97	0.45
1:A:323:LYS:O	1:A:327:ILE:HG13	2.18	0.44
1:A:190:LEU:HD23	1:A:190:LEU:C	2.42	0.44
1:B:382:SER:CB	1:B:386:LEU:HG	2.47	0.44
1:B:179:THR:HG22	1:B:374:SER:HA	1.92	0.44
1:B:351:ILE:HG12	1:B:379:SER:HG	1.79	0.44
1:A:233:THR:HG23	1:A:474:ASP:OD1	2.17	0.44
1:A:382:SER:OG	1:A:386:LEU:HD12	2.18	0.44
1:B:382:SER:HB2	1:B:386:LEU:HG	2.00	0.44
1:A:190:LEU:C	1:A:190:LEU:CD2	2.91	0.44
1:B:330:LYS:HB2	1:B:330:LYS:HZ2	1.82	0.44
1:B:40:ARG:HD2	1:B:398:SER:CB	2.48	0.44
1:A:88:ARG:HG3	1:A:88:ARG:HH11	1.82	0.43
1:A:434:ARG:HB2	1:A:434:ARG:NH1	2.33	0.43
1:B:41:GLU:HG3	1:B:423:LYS:HG3	1.99	0.43
1:B:15:THR:HG22	1:B:16:ASP:N	2.33	0.43
1:A:114:ILE:CD1	1:A:148:ILE:HD13	2.46	0.43
1:A:283:ILE:HG12	1:A:284:TYR:N	2.33	0.43
1:A:383:GLY:C	1:A:385:ALA:H	2.26	0.43
1:A:77:LYS:HG2	1:A:105:LEU:HD21	1.99	0.43
1:A:450:LEU:HB2	1:A:452:GLU:HG3	2.00	0.43
1:B:432:LEU:HD23	1:B:433:HIS:H	1.78	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:ASP:O	1:A:323:LYS:HG3	2.19	0.43
1:A:309:ILE:HG21	1:A:351:ILE:CD1	2.48	0.42
1:A:176:LEU:HD23	1:A:176:LEU:O	2.19	0.42
1:A:481:GLN:HE21	1:A:482:LEU:H	1.68	0.42
1:B:330:LYS:NZ	1:B:330:LYS:CB	2.80	0.42
1:A:434:ARG:NH1	1:A:434:ARG:CB	2.82	0.42
1:A:435:THR:HG22	1:A:453:TYR:CD2	2.55	0.42
1:B:291:TRP:HA	1:B:291:TRP:CE3	2.54	0.42
1:B:295:LEU:HD12	1:B:295:LEU:N	2.33	0.42
1:B:309:ILE:HG21	1:B:351:ILE:HG13	2.00	0.42
1:A:148:ILE:O	1:A:151:ILE:HG22	2.19	0.42
1:B:427:LYS:O	1:B:444:GLU:HB3	2.19	0.42
1:B:168:GLN:NE2	1:B:386:LEU:HD21	2.34	0.42
1:A:358:ILE:HG23	1:A:359:ASN:N	2.35	0.42
1:B:278:SER:OG	1:B:310:ILE:HG23	2.20	0.42
1:B:336:GLU:HG2	1:B:340:GLY:HA2	2.02	0.42
1:A:481:GLN:NE2	1:A:482:LEU:H	2.17	0.41
1:A:151:ILE:HG23	1:A:152:LEU:N	2.35	0.41
1:A:384:GLY:O	1:A:388:GLN:HB3	2.20	0.41
1:B:62:LEU:HD22	1:B:66:LEU:HG	2.02	0.41
1:B:179:THR:HG22	1:B:179:THR:O	2.19	0.41
1:A:311:ARG:HA	1:A:312:PRO:HD2	1.78	0.41
1:A:17:SER:O	1:A:20:VAL:HG23	2.20	0.41
1:A:173:ALA:HB2	1:A:186:LEU:HD11	2.02	0.41
1:A:312:PRO:CB	1:A:324:VAL:HG21	2.46	0.41
1:B:483:ASN:O	1:B:485:GLU:HG3	2.21	0.41
1:A:255:LYS:HG3	1:A:256:ASP:N	2.35	0.41
1:A:33:VAL:HG13	1:A:33:VAL:O	2.20	0.41
1:A:324:VAL:O	1:A:328:LEU:HG	2.20	0.41
1:A:56:GLU:HA	1:A:126:PRO:HA	2.02	0.41
1:A:78:GLU:H	1:A:78:GLU:CD	2.29	0.41
1:A:86:VAL:HG11	1:B:221:VAL:CG1	2.49	0.41
1:A:272:VAL:HB	1:A:273:PRO:HD2	2.02	0.41
1:A:378:VAL:HG12	1:A:379:SER:N	2.35	0.41
1:B:18:TYR:CD1	1:B:18:TYR:C	2.99	0.41
1:A:11:ILE:HG23	1:A:12:LEU:HD23	2.03	0.41
1:A:23:TYR:CD2	1:A:97:ASN:HB2	2.56	0.41
1:A:168:GLN:NE2	1:A:386:LEU:CD1	2.80	0.41
1:B:226:LEU:HD23	1:B:226:LEU:C	2.46	0.41
1:A:143:TRP:CD1	1:A:143:TRP:H	2.39	0.40
1:B:168:GLN:HE22	1:B:386:LEU:CD1	2.28	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:HIS:CE1	1:B:219:ASP:OD1	2.70	0.40
1:A:352:GLN:NE2	1:A:354:ASP:H	2.19	0.40
1:B:179:THR:HG23	1:B:341:TYR:CD2	2.57	0.40
1:A:411:VAL:HG12	1:A:412:ASN:N	2.35	0.40
1:B:432:LEU:HD23	1:B:432:LEU:C	2.47	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	450/491 (92%)	432 (96%)	17 (4%)	1 (0%)	43	36
1	B	454/491 (92%)	442 (97%)	10 (2%)	2 (0%)	30	22
All	All	904/982 (92%)	874 (97%)	27 (3%)	3 (0%)	36	29

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	455	HIS
1	B	293	GLU
1	A	312	PRO

5.3.2 Protein sidechains [i](#)

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	402/431 (93%)	389 (97%)	13 (3%)	34	27
1	B	406/431 (94%)	394 (97%)	12 (3%)	36	30
All	All	808/862 (94%)	783 (97%)	25 (3%)	35	29

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	GLU
1	A	12	LEU
1	A	53	LYS
1	A	127	ARG
1	A	144	LEU
1	A	186	LEU
1	A	259	LYS
1	A	283	ILE
1	A	330	LYS
1	A	331	LYS
1	A	366	GLU
1	A	396	ASN
1	A	432	LEU
1	B	8	GLU
1	B	12	LEU
1	B	62	LEU
1	B	144	LEU
1	B	186	LEU
1	B	187	GLU
1	B	219	ASP
1	B	330	LYS
1	B	343	LEU
1	B	361	LEU
1	B	366	GLU
1	B	386	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	GLN
1	A	90	HIS
1	A	111	HIS
1	A	129	ASN
1	A	168	GLN

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Mol	Chain	Res	Type
1	A	182	ASN
1	A	191	HIS
1	A	201	GLN
1	A	214	ASN
1	A	247	HIS
1	A	352	GLN
1	A	396	ASN
1	A	481	GLN
1	B	22	HIS
1	B	67	ASN
1	B	81	GLN
1	B	90	HIS
1	B	111	HIS
1	B	154	GLN
1	B	164	ASN
1	B	168	GLN
1	B	182	ASN
1	B	191	HIS
1	B	201	GLN
1	B	247	HIS
1	B	352	GLN
1	B	362	GLN
1	B	388	GLN
1	B	412	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	456/491 (92%)	0.89	77 (16%) 4 4	15, 31, 63, 82	0
1	B	460/491 (93%)	0.70	63 (13%) 6 7	14, 28, 61, 87	0
All	All	916/982 (93%)	0.79	140 (15%) 5 5	14, 30, 63, 87	0

All (140) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	386	LEU	10.7
1	B	386	LEU	9.9
1	B	282	ASP	8.7
1	B	283	ILE	8.6
1	B	387	LEU	8.1
1	B	454	GLY	8.1
1	A	283	ILE	7.1
1	A	387	LEU	6.2
1	A	452	GLU	6.1
1	A	52	VAL	5.8
1	B	292	GLY	5.6
1	A	284	TYR	5.4
1	A	413	VAL	5.2
1	B	385	ALA	4.9
1	B	313	ASP	4.8
1	A	295	LEU	4.8
1	B	285	ASN	4.8
1	B	286	ALA	4.5
1	A	385	ALA	4.5
1	B	388	GLN	4.4
1	B	485	GLU	4.4
1	B	412	ASN	4.4
1	A	288	GLU	4.4
1	B	281	TYR	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	388	GLN	4.2
1	B	455	HIS	4.1
1	B	295	LEU	4.1
1	A	286	ALA	4.1
1	B	411	VAL	4.0
1	A	279	ASP	4.0
1	B	43	LYS	4.0
1	A	365	VAL	4.0
1	A	409	LEU	3.9
1	B	284	TYR	3.8
1	A	53	LYS	3.8
1	B	296	ARG	3.8
1	B	484	MET	3.7
1	A	281	TYR	3.7
1	A	323	LYS	3.7
1	A	453	TYR	3.6
1	A	311	ARG	3.5
1	A	178	GLU	3.5
1	A	411	VAL	3.5
1	A	293	GLU	3.5
1	A	282	ASP	3.5
1	B	294	ASP	3.5
1	A	285	ASN	3.3
1	B	287	CYS	3.3
1	B	290	ILE	3.3
1	A	455	HIS	3.3
1	B	288	GLU	3.2
1	B	384	GLY	3.2
1	A	313	ASP	3.2
1	B	293	GLU	3.2
1	A	450	LEU	3.1
1	B	18	TYR	3.1
1	A	179	THR	3.1
1	B	311	ARG	3.1
1	A	314	SER	3.1
1	A	300	VAL	3.1
1	A	454	GLY	3.1
1	A	290	ILE	3.0
1	B	383	GLY	3.0
1	B	312	PRO	3.0
1	A	410	GLY	2.9
1	B	327	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	247	HIS	2.9
1	A	289	LYS	2.9
1	A	370	GLN	2.8
1	B	259	LYS	2.8
1	B	309	ILE	2.8
1	A	42	LYS	2.8
1	A	335	SER	2.8
1	A	312	PRO	2.8
1	B	300	VAL	2.8
1	A	18	TYR	2.7
1	B	483	ASN	2.7
1	A	292	GLY	2.7
1	A	287	CYS	2.7
1	B	421	PRO	2.7
1	B	453	TYR	2.6
1	A	176	LEU	2.6
1	A	95	VAL	2.6
1	A	175	TYR	2.6
1	A	384	GLY	2.6
1	A	371	LYS	2.6
1	B	266	VAL	2.6
1	A	412	ASN	2.5
1	A	483	ASN	2.5
1	B	382	SER	2.5
1	A	182	ASN	2.5
1	A	94	ASP	2.5
1	B	209	SER	2.5
1	B	354	ASP	2.5
1	B	450	LEU	2.4
1	B	280	SER	2.4
1	A	339	LYS	2.4
1	B	326	ASP	2.4
1	A	255	LYS	2.4
1	A	351	ILE	2.4
1	A	360	THR	2.4
1	A	318	LEU	2.4
1	A	481	GLN	2.4
1	B	436	PRO	2.4
1	B	297	HIS	2.4
1	A	99	ARG	2.3
1	A	343	LEU	2.3
1	A	341	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	254	GLY	2.3
1	A	425	SER	2.3
1	A	324	VAL	2.3
1	A	389	LYS	2.3
1	B	314	SER	2.3
1	B	437	ALA	2.2
1	B	272	VAL	2.2
1	A	333	PRO	2.2
1	A	367	GLY	2.2
1	A	372	LYS	2.2
1	A	296	ARG	2.2
1	A	177	LEU	2.2
1	B	240	TYR	2.2
1	B	269	PHE	2.2
1	B	277	VAL	2.2
1	A	233	THR	2.2
1	A	338	SER	2.2
1	A	330	LYS	2.2
1	B	336	GLU	2.1
1	A	315	GLY	2.1
1	B	55	GLU	2.1
1	B	332	PHE	2.1
1	A	378	VAL	2.1
1	B	298	LEU	2.1
1	A	354	ASP	2.1
1	B	179	THR	2.1
1	B	360	THR	2.1
1	A	448	GLY	2.1
1	B	333	PRO	2.1
1	A	369	LYS	2.0
1	B	346	PRO	2.0
1	B	323	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides 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.