Full wwPDB X-ray Structure Validation Report (i)

Jun 11, 2024 – 07:39 PM EDT

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PDB ID	:	2G95
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)

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	Percentile Ranks	Value
Rfree		0.267
Clashscore		16
Ramachandran outliers		0.3%
Sidechain outliers		3.0%
RSRZ outliers		6.3%

Worse *Better*

∎ Percentile relative to all X-ray structures

◻ Percentile relative to X-ray structures of similar resolution
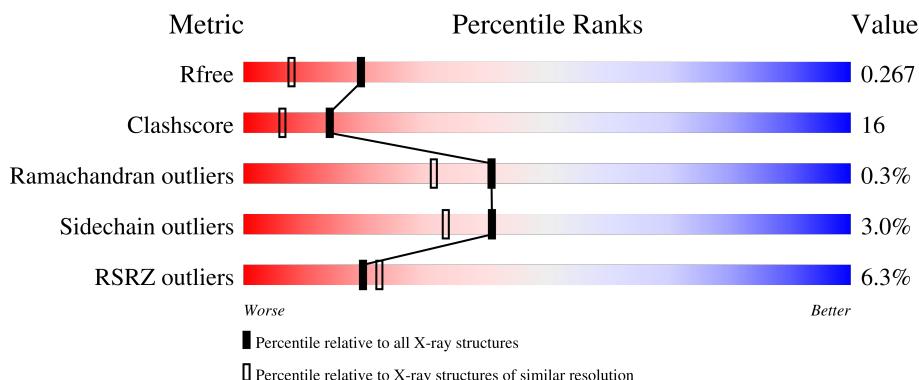
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 <=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	5% — 64% / 27% / • 7%
1	B	491	6% — 68% / 24% / • 6%
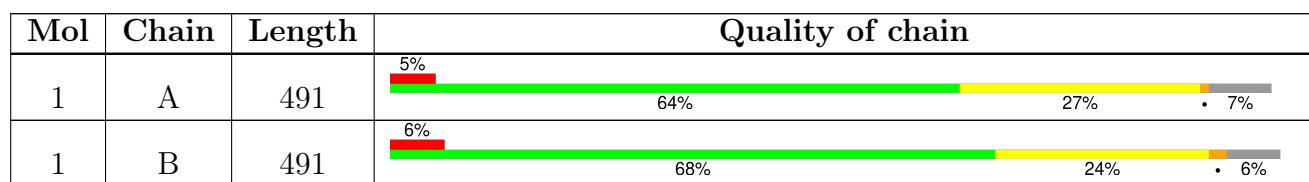
2 Entry composition ⓘ

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 3644	C 2339	N 605	O 694	S 6	0	0	0
1	B	460	Total 3682	C 2360	N 614	O 701	S 7	0	0	0

- Molecule 2 is water.

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

3 Residue-property plots ⓘ

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

Chain A:

• Molecule 1: Nicotinamide phosphoribosyltransferase

Chain B:
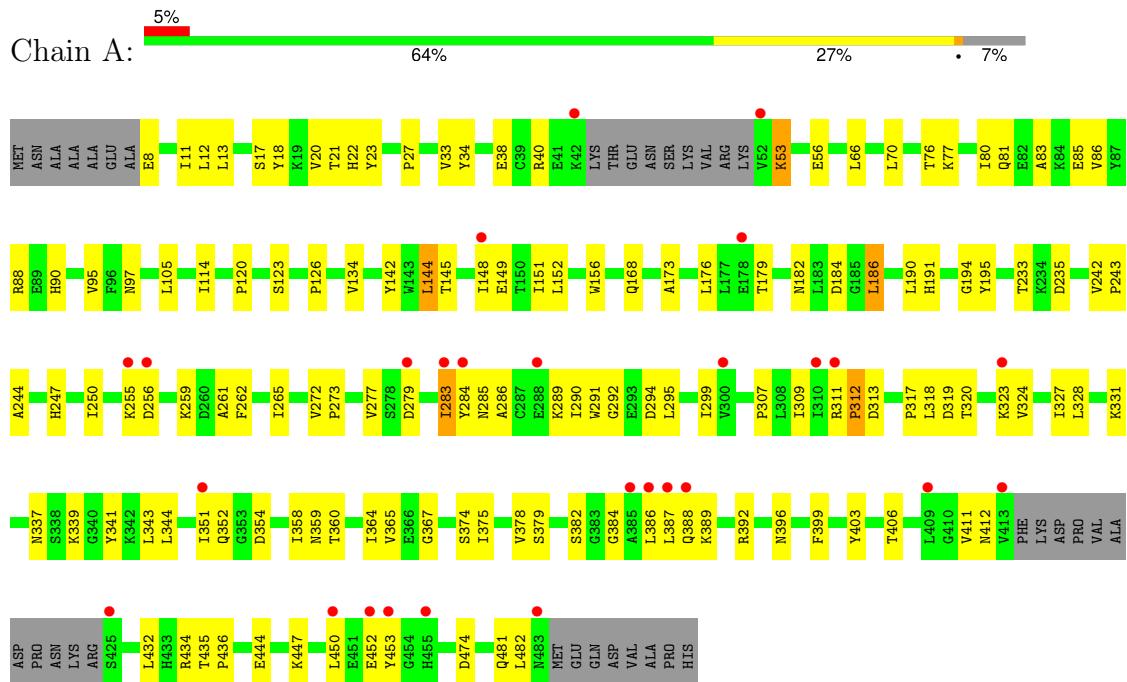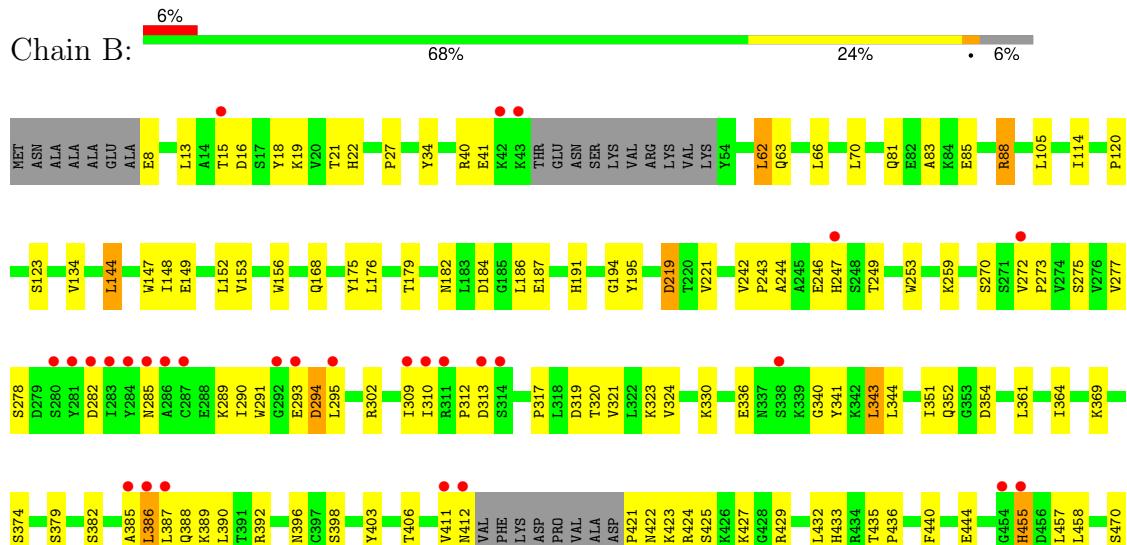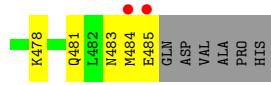
4 Data and refinement statistics ⓘ

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 31.03 – 1.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-1.90) 95.1 (31.03-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (Å²)	23.0	Xtriage
Anisotropy	0.525	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.36 , 48.4	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	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 (Å²)	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.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.34	0/3728	0.57	0/5051
1	B	0.35	0/3767	0.59	0/5100
All	All	0.34	0/7495	0.58	0/10151

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	3644	0	3615	132	0
1	B	3682	0	3652	104	0
2	A	104	0	0	1	0
2	B	147	0	0	1	0
All	All	7577	0	7267	228	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 (228) 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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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:B:105:LEU:C	1:B:105:LEU:HD23	2.25	0.56
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:ASP:C	1:A:295:LEU:HD12	2.29	0.54
1:B:168:GLN:HE22	1:B:386:LEU:HD21	1.71	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: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
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:B:294:ASP:C	1:B:295:LEU:HD12	2.33	0.49
1:A:17:SER:OG	1:A:90:HIS:HE1	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:88:ARG:HD3	1:B:88:ARG:C	2.33	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
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: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:A:312:PRO:HD2	1:A:351:ILE:O	2.16	0.45
1:B:15:THR:OG1	1:B:147:TRP:CD1	2.68	0.45
1:B:429:ARG:HH11	1:B:429:ARG:HG3	1.81	0.45
1:B:330:LYS:HB2	1:B:330:LYS:HZ2	1.80	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:B:351:ILE:HG12	1:B:379:SER:HG	1.80	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
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:B:388:GLN:C	1:B:390:LEU:H	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:38:GLU:CD	1:A:40:ARG:HG2	2.42	0.41
1:A:56:GLU:HA	1:A:126:PRO:HA	2.02	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: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:168:GLN:HE22	1:B:386:LEU:CD1	2.28	0.40
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

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	450/491 (92%)	432 (96%)	17 (4%)	1 (0%)	47	38
1	B	454/491 (92%)	442 (97%)	10 (2%)	2 (0%)	34	24
All	All	904/982 (92%)	874 (97%)	27 (3%)	3 (0%)	41	31

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 ⓘ

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%)	393 (98%)	9 (2%)	52	47
1	B	406/431 (94%)	391 (96%)	15 (4%)	34	25
All	All	808/862 (94%)	784 (97%)	24 (3%)	41	33

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

Mol	Chain	Res	Type
1	A	8	GLU
1	A	22	HIS
1	A	53	LYS
1	A	144	LEU
1	A	186	LEU
1	A	195	TYR
1	A	283	ILE
1	A	396	ASN
1	A	432	LEU
1	B	8	GLU
1	B	22	HIS
1	B	62	LEU
1	B	88	ARG
1	B	144	LEU
1	B	186	LEU
1	B	187	GLU
1	B	195	TYR
1	B	219	ASP
1	B	294	ASP
1	B	343	LEU

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Mol	Chain	Res	Type
1	B	361	LEU
1	B	386	LEU
1	B	396	ASN
1	B	484	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	GLN
1	A	90	HIS
1	A	111	HIS
1	A	168	GLN
1	A	182	ASN
1	A	191	HIS
1	A	247	HIS
1	A	352	GLN
1	A	362	GLN
1	A	396	ASN
1	A	481	GLN
1	B	22	HIS
1	B	81	GLN
1	B	90	HIS
1	B	111	HIS
1	B	146	ASN
1	B	164	ASN
1	B	168	GLN
1	B	182	ASN
1	B	191	HIS
1	B	211	HIS
1	B	247	HIS
1	B	352	GLN
1	B	388	GLN

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 (i)

There are no monosaccharides 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	456/491 (92%)	0.38	27 (5%)	22	25	15, 31, 63, 82	0
1	B	460/491 (93%)	0.33	31 (6%)	17	20	14, 28, 61, 87	0
All	All	916/982 (93%)	0.35	58 (6%)	20	22	14, 30, 63, 87	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	386	LEU	9.8
1	B	386	LEU	8.6
1	A	52	VAL	8.1
1	B	454	GLY	7.9
1	B	282	ASP	7.1
1	A	452	GLU	7.0
1	B	387	LEU	6.2
1	B	313	ASP	5.6
1	B	484	MET	5.5
1	B	485	GLU	5.4
1	A	42	LYS	5.2
1	B	311	ARG	4.1
1	B	284	TYR	3.9
1	B	314	SER	3.7
1	A	450	LEU	3.4
1	A	453	TYR	3.4
1	A	311	ARG	3.3
1	A	455	HIS	3.3
1	A	413	VAL	3.3
1	A	387	LEU	3.2
1	A	385	ALA	3.2
1	B	293	GLU	3.2
1	A	409	LEU	3.0
1	B	385	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	292	GLY	2.9
1	B	310	ILE	2.9
1	B	411	VAL	2.9
1	B	281	TYR	2.8
1	A	351	ILE	2.8
1	A	148	ILE	2.7
1	A	323	LYS	2.6
1	B	309	ILE	2.6
1	B	283	ILE	2.6
1	B	285	ASN	2.5
1	A	284	TYR	2.5
1	B	412	ASN	2.5
1	B	280	SER	2.4
1	B	272	VAL	2.4
1	A	288	GLU	2.4
1	A	178	GLU	2.4
1	A	283	ILE	2.3
1	B	287	CYS	2.3
1	B	247	HIS	2.3
1	A	388	GLN	2.2
1	A	300	VAL	2.2
1	B	286	ALA	2.2
1	B	455	HIS	2.2
1	A	483	ASN	2.2
1	A	425	SER	2.2
1	B	15	THR	2.2
1	B	43	LYS	2.2
1	A	279	ASP	2.2
1	A	255	LYS	2.1
1	A	310	ILE	2.1
1	B	42	LYS	2.1
1	B	295	LEU	2.1
1	A	256	ASP	2.1
1	B	338	SER	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides 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.