



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:15 PM GMT

PDB ID : 1JI1
Title : Crystal Structure Analysis of Thermoactinomyces vulgaris R-47 alpha-Amylase 1
Authors : Kamitori, S.; Abe, A.; Ohtaki, A.; Kaji, A.; Tonozuka, T.; Sakano, Y.
Deposited on : 2001-06-28
Resolution : 1.60 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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

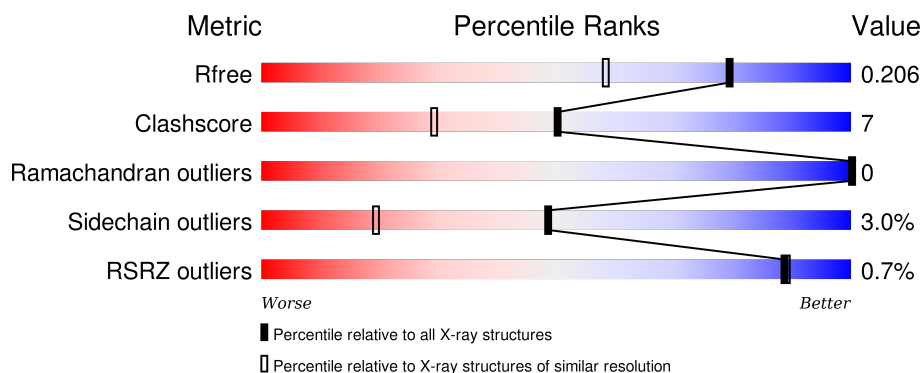
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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}	91344	2475 (1.60-1.60)
Clashscore	102246	2732 (1.60-1.60)
Ramachandran outliers	100387	2654 (1.60-1.60)
Sidechain outliers	100360	2653 (1.60-1.60)
RSRZ outliers	91569	2479 (1.60-1.60)

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	637	<div> <div></div> <div>86%12%•</div> </div>
1	B	637	<div> <div></div> <div>87%11%•</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11556 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 ALPHA-AMYLASE I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	637	Total	C	N	O	S	0	0	0
			5038	3192	842	994	10			
1	B	637	Total	C	N	O	S	0	0	0
			5038	3192	842	994	10			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total	Ca	0	0
			3	3		
2	A	3	Total	Ca	0	0
			3	3		

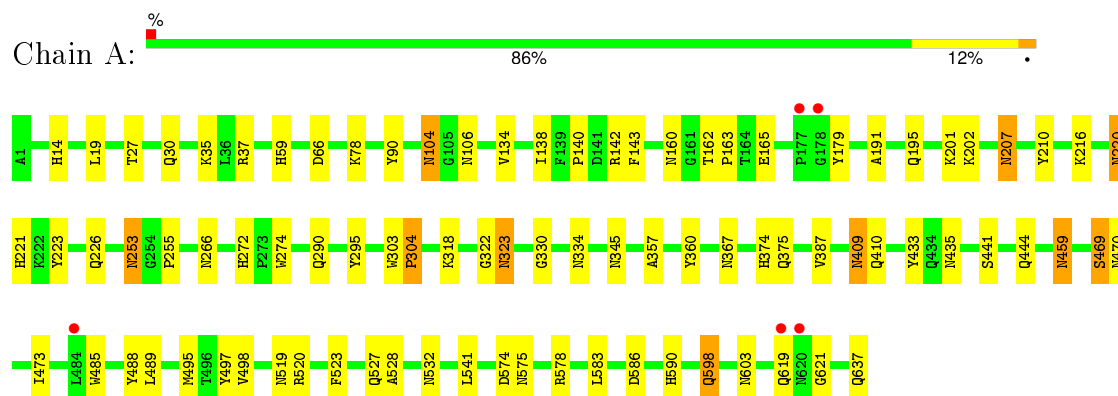
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	725	Total	O	0	0
			725	725		
3	B	749	Total	O	0	0
			749	749		

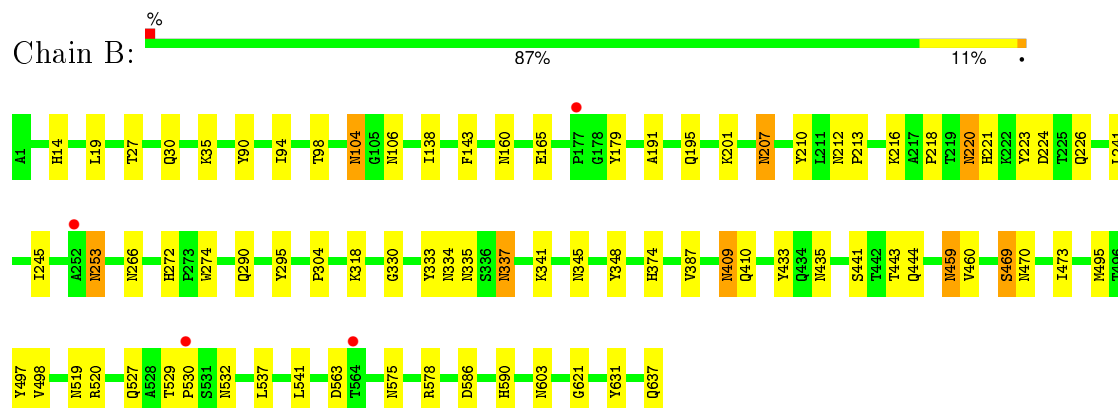
3 Residue-property plots [i](#)

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: ALPHA-AMYLASE I



• Molecule 1: ALPHA-AMYLASE I



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	122.57Å 50.84Å 107.80Å 90.00° 104.20° 90.00°	Depositor
Resolution (Å)	20.46 – 1.60 20.46 – 1.50	Depositor EDS
% Data completeness (in resolution range)	89.7 (20.46-1.60) 86.8 (20.46-1.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.35 (at 1.50Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.182 , 0.206 0.182 , 0.206	Depositor DCC
R_{free} test set	15156 reflections (9.92%)	DCC
Wilson B-factor (Å ²)	10.7	Xtriage
Anisotropy	0.394	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 39.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	2 of 179079 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11556	wwPDB-VP
Average B, all atoms (Å ²)	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 82.79 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.5569e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	0.31	0/5195	0.61	0/7108
1	B	0.31	0/5195	0.62	0/7108
All	All	0.31	0/10390	0.62	0/14216

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	5038	0	4648	76	0
1	B	5038	0	4648	61	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	725	0	0	4	0
3	B	749	0	0	2	0
All	All	11556	0	9296	135	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 7.

All (135) 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:527:GLN:HE21	1:A:532:ASN:HD22	1.03	0.95
1:B:578:ARG:HE	1:B:637:GLN:HE21	1.11	0.91
1:A:578:ARG:HE	1:A:637:GLN:HE21	1.19	0.91
1:A:272:HIS:HD2	1:A:274:TRP:H	1.19	0.91
1:B:272:HIS:HD2	1:B:274:TRP:H	1.19	0.89
1:A:603:ASN:HD21	1:A:621:GLY:H	1.20	0.88
1:B:603:ASN:HD21	1:B:621:GLY:H	1.22	0.83
1:B:441:SER:H	1:B:444:GLN:HE21	1.30	0.77
1:A:37:ARG:HH22	1:A:598:GLN:HE22	1.33	0.75
1:A:207:ASN:H	1:A:207:ASN:HD22	1.35	0.74
1:A:441:SER:H	1:A:444:GLN:HE21	1.36	0.74
1:B:207:ASN:H	1:B:207:ASN:HD22	1.35	0.73
1:A:527:GLN:NE2	1:A:532:ASN:HD22	1.83	0.72
1:B:221:HIS:HD2	1:B:223:TYR:H	1.37	0.72
1:B:578:ARG:HE	1:B:637:GLN:NE2	1.86	0.72
1:A:603:ASN:ND2	1:A:621:GLY:H	1.88	0.71
1:A:221:HIS:HD2	1:A:223:TYR:H	1.37	0.71
1:A:27:THR:H	1:A:30:GLN:HE21	1.39	0.70
1:A:603:ASN:HD21	1:A:621:GLY:N	1.89	0.69
1:B:603:ASN:ND2	1:B:621:GLY:H	1.90	0.69
1:A:216:LYS:HE3	1:A:226:GLN:NE2	2.09	0.68
1:A:221:HIS:CD2	1:A:223:TYR:H	2.13	0.66
1:A:527:GLN:HE21	1:A:532:ASN:ND2	1.86	0.66
1:B:221:HIS:CD2	1:B:223:TYR:H	2.14	0.64
1:B:603:ASN:HD21	1:B:621:GLY:N	1.93	0.64
1:A:59:HIS:HD2	1:B:98:THR:O	1.81	0.64
1:A:323:ASN:HD22	1:A:323:ASN:N	1.96	0.63
1:B:220:ASN:HD22	1:B:221:HIS:N	1.97	0.62
1:A:374:HIS:HD2	1:A:410:GLN:OE1	1.83	0.62
1:A:441:SER:H	1:A:444:GLN:NE2	1.97	0.61
1:B:441:SER:H	1:B:444:GLN:NE2	1.98	0.59
1:A:586:ASP:OD1	1:A:590:HIS:HE1	1.86	0.58
1:B:374:HIS:HD2	1:B:410:GLN:OE1	1.87	0.58
1:A:357:ALA:HB2	3:A:2498:HOH:O	2.02	0.58
1:A:220:ASN:HD22	1:A:221:HIS:N	2.02	0.58
1:A:216:LYS:HE3	1:A:226:GLN:HE21	1.70	0.57
1:A:409:ASN:HD21	1:A:410:GLN:HE21	1.51	0.56
1:B:165:GLU:HB2	1:B:179:TYR:CD2	2.40	0.56
1:A:578:ARG:HE	1:A:637:GLN:NE2	1.96	0.56
1:B:345:ASN:ND2	1:B:387:VAL:HG13	2.21	0.56
1:A:19:LEU:HD21	1:A:574:ASP:C	2.26	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:578:ARG:NE	1:B:637:GLN:HE21	1.92	0.55
1:A:202:LYS:HE3	1:A:253:ASN:O	2.07	0.54
1:A:485:TRP:HA	1:A:488:TYR:CD1	2.42	0.54
1:B:14:HIS:HD2	1:B:35:LYS:O	1.91	0.54
1:A:165:GLU:HB2	1:A:179:TYR:CD2	2.43	0.54
1:B:266:ASN:HD21	1:B:318:LYS:HE2	1.73	0.54
1:B:253:ASN:HD22	1:B:253:ASN:H	1.55	0.53
1:A:266:ASN:HD21	1:A:318:LYS:HE2	1.73	0.53
1:B:337:ASN:HD22	1:B:337:ASN:H	1.57	0.52
1:A:14:HIS:HD2	1:A:35:LYS:O	1.92	0.52
1:A:201:LYS:NZ	1:A:253:ASN:HD21	2.07	0.52
1:A:253:ASN:H	1:A:253:ASN:HD22	1.57	0.52
1:B:104:ASN:ND2	1:B:106:ASN:H	2.06	0.52
1:B:253:ASN:ND2	1:B:253:ASN:H	2.07	0.52
1:A:66:ASP:HB2	1:A:78:LYS:HG2	1.92	0.52
1:A:459:ASN:N	1:A:459:ASN:HD22	2.08	0.51
1:B:469:SER:HA	1:B:473:ILE:HD11	1.92	0.51
1:B:409:ASN:HD21	1:B:410:GLN:HE21	1.59	0.51
1:B:495:MET:HG3	1:B:541:LEU:HB3	1.93	0.51
1:B:586:ASP:OD1	1:B:590:HIS:HE1	1.94	0.51
1:A:345:ASN:ND2	1:A:387:VAL:HG13	2.26	0.50
1:A:374:HIS:HE1	3:A:2587:HOH:O	1.94	0.50
1:B:409:ASN:H	1:B:409:ASN:HD22	1.58	0.50
1:A:330:GLY:HA2	1:A:334:ASN:HB2	1.93	0.50
1:A:104:ASN:ND2	1:A:106:ASN:H	2.09	0.50
1:B:27:THR:H	1:B:30:GLN:HE21	1.60	0.49
1:A:409:ASN:H	1:A:409:ASN:HD22	1.58	0.49
1:B:104:ASN:C	1:B:104:ASN:HD22	2.16	0.49
1:A:495:MET:HG3	1:A:541:LEU:HB3	1.93	0.49
1:B:138:ILE:HG23	1:B:143:PHE:HB2	1.94	0.49
1:B:290:GLN:HA	1:B:295:TYR:CD1	2.48	0.49
1:A:14:HIS:HE1	1:A:90:TYR:OH	1.96	0.48
1:A:37:ARG:NH2	1:A:598:GLN:HE22	2.05	0.48
1:A:134:VAL:H	1:A:207:ASN:ND2	2.12	0.48
1:A:37:ARG:HH22	1:A:598:GLN:NE2	2.08	0.47
1:B:374:HIS:HE1	3:B:2673:HOH:O	1.97	0.47
1:A:253:ASN:H	1:A:253:ASN:ND2	2.12	0.47
1:B:337:ASN:N	1:B:337:ASN:HD22	2.12	0.47
1:B:253:ASN:HD22	1:B:253:ASN:N	2.12	0.47
1:B:459:ASN:N	1:B:459:ASN:HD22	2.12	0.47
1:A:191:ALA:O	1:A:195:GLN:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:LYS:HE3	1:B:226:GLN:OE1	2.15	0.47
1:A:469:SER:HA	1:A:473:ILE:HD11	1.96	0.46
1:A:207:ASN:N	1:A:207:ASN:HD22	2.05	0.46
1:B:519:ASN:OD1	1:B:520:ARG:HG3	2.16	0.46
1:A:290:GLN:HA	1:A:295:TYR:CD1	2.51	0.46
1:B:335:ASN:HB3	1:B:337:ASN:ND2	2.29	0.46
1:B:207:ASN:N	1:B:207:ASN:HD22	2.03	0.46
1:B:459:ASN:HD22	1:B:460:VAL:H	1.63	0.46
1:B:443:THR:HG23	1:B:563:ASP:OD1	2.15	0.46
1:B:330:GLY:HA2	1:B:334:ASN:HB2	1.98	0.46
1:A:323:ASN:N	1:A:323:ASN:ND2	2.63	0.45
1:A:19:LEU:HD22	1:A:575:ASN:ND2	2.31	0.45
1:B:14:HIS:HE1	1:B:90:TYR:OH	1.99	0.45
1:A:104:ASN:HD22	1:A:104:ASN:C	2.20	0.45
1:A:489:LEU:HD11	1:A:583:LEU:HB3	1.99	0.44
1:A:497:TYR:CG	1:A:498:VAL:N	2.86	0.44
1:A:59:HIS:CD2	1:B:98:THR:O	2.67	0.44
1:A:621:GLY:HA2	3:A:2228:HOH:O	2.17	0.44
1:A:253:ASN:HD22	1:A:253:ASN:N	2.14	0.44
1:A:138:ILE:O	1:A:140:PRO:HD3	2.18	0.44
1:A:142:ARG:HG3	1:A:520:ARG:O	2.18	0.44
1:A:519:ASN:OD1	1:A:520:ARG:HG3	2.18	0.44
1:B:497:TYR:CG	1:B:498:VAL:N	2.85	0.43
1:A:523:PHE:CE1	1:A:528:ALA:HB2	2.53	0.43
1:B:527:GLN:NE2	1:B:532:ASN:HD22	2.17	0.43
1:A:201:LYS:HE3	1:A:255:PRO:O	2.18	0.43
1:B:19:LEU:HD23	1:B:575:ASN:ND2	2.33	0.43
1:B:191:ALA:O	1:B:195:GLN:HG3	2.19	0.43
1:B:621:GLY:HA2	3:B:2190:HOH:O	2.19	0.43
1:B:409:ASN:ND2	1:B:410:GLN:HG3	2.34	0.43
1:A:441:SER:N	1:A:444:GLN:HE21	2.12	0.43
1:B:345:ASN:HD21	1:B:387:VAL:HG13	1.84	0.43
1:B:218:PRO:HG2	1:B:224:ASP:OD2	2.18	0.43
1:A:619:GLN:HG2	3:A:2536:HOH:O	2.18	0.43
1:B:245:ILE:HG21	1:B:348:TYR:O	2.19	0.43
1:A:134:VAL:H	1:A:207:ASN:HD21	1.66	0.42
1:B:333:TYR:O	1:B:341:LYS:HE3	2.19	0.42
1:A:603:ASN:HD22	1:A:603:ASN:HA	1.68	0.42
1:A:322:GLY:C	1:A:323:ASN:HD22	2.23	0.42
1:B:529:THR:HB	1:B:530:PRO:HD2	2.01	0.42
1:B:94:ILE:N	1:B:94:ILE:HD12	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:THR:HA	1:A:163:PRO:HD3	1.85	0.42
1:B:272:HIS:CD2	1:B:274:TRP:H	2.12	0.42
1:B:201:LYS:NZ	1:B:253:ASN:HD21	2.18	0.42
1:A:360:TYR:HD2	1:A:367:ASN:ND2	2.18	0.41
1:A:409:ASN:N	1:A:409:ASN:HD22	2.17	0.41
1:A:19:LEU:HD13	1:A:575:ASN:ND2	2.35	0.41
1:A:138:ILE:HG23	1:A:143:PHE:HB2	2.02	0.40
1:A:19:LEU:CD2	1:A:574:ASP:C	2.89	0.40
1:A:345:ASN:HD22	1:A:345:ASN:HA	1.75	0.40
1:B:241:LEU:O	1:B:245:ILE:HG13	2.21	0.40
1:A:303:TRP:HA	1:A:304:PRO:HA	1.85	0.40
1:B:212:ASN:HB3	1:B:213:PRO:HD2	2.03	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	635/637 (100%)	617 (97%)	18 (3%)	0	100	100
1	B	635/637 (100%)	616 (97%)	19 (3%)	0	100	100
All	All	1270/1274 (100%)	1233 (97%)	37 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	540/540 (100%)	524 (97%)	16 (3%)	48	19
1	B	540/540 (100%)	524 (97%)	16 (3%)	48	19
All	All	1080/1080 (100%)	1048 (97%)	32 (3%)	48	19

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	ASN
1	A	160	ASN
1	A	207	ASN
1	A	210	TYR
1	A	220	ASN
1	A	253	ASN
1	A	304	PRO
1	A	323	ASN
1	A	375	GLN
1	A	409	ASN
1	A	433	TYR
1	A	435	ASN
1	A	459	ASN
1	A	469	SER
1	A	470	ASN
1	A	598	GLN
1	B	104	ASN
1	B	160	ASN
1	B	207	ASN
1	B	210	TYR
1	B	220	ASN
1	B	253	ASN
1	B	304	PRO
1	B	337	ASN
1	B	409	ASN
1	B	433	TYR
1	B	435	ASN
1	B	459	ASN
1	B	469	SER
1	B	470	ASN
1	B	537	LEU
1	B	631	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (87) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	14	HIS
1	A	30	GLN
1	A	56	ASN
1	A	59	HIS
1	A	68	ASN
1	A	104	ASN
1	A	123	ASN
1	A	137	GLN
1	A	153	GLN
1	A	160	ASN
1	A	195	GLN
1	A	207	ASN
1	A	220	ASN
1	A	221	HIS
1	A	226	GLN
1	A	253	ASN
1	A	266	ASN
1	A	272	HIS
1	A	280	ASN
1	A	314	ASN
1	A	323	ASN
1	A	345	ASN
1	A	364	ASN
1	A	367	ASN
1	A	374	HIS
1	A	375	GLN
1	A	407	GLN
1	A	409	ASN
1	A	410	GLN
1	A	435	ASN
1	A	444	GLN
1	A	459	ASN
1	A	461	GLN
1	A	494	GLN
1	A	512	GLN
1	A	527	GLN
1	A	539	GLN
1	A	546	ASN
1	A	575	ASN
1	A	585	ASN
1	A	590	HIS

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Mol	Chain	Res	Type
1	A	598	GLN
1	A	603	ASN
1	A	614	HIS
1	A	637	GLN
1	B	6	ASN
1	B	10	ASN
1	B	14	HIS
1	B	30	GLN
1	B	68	ASN
1	B	104	ASN
1	B	123	ASN
1	B	137	GLN
1	B	153	GLN
1	B	160	ASN
1	B	195	GLN
1	B	207	ASN
1	B	220	ASN
1	B	221	HIS
1	B	253	ASN
1	B	266	ASN
1	B	272	HIS
1	B	280	ASN
1	B	337	ASN
1	B	345	ASN
1	B	364	ASN
1	B	374	HIS
1	B	407	GLN
1	B	409	ASN
1	B	410	GLN
1	B	435	ASN
1	B	436	ASN
1	B	444	GLN
1	B	459	ASN
1	B	494	GLN
1	B	512	GLN
1	B	527	GLN
1	B	539	GLN
1	B	546	ASN
1	B	575	ASN
1	B	585	ASN
1	B	590	HIS
1	B	593	ASN

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Mol	Chain	Res	Type
1	B	603	ASN
1	B	614	HIS
1	B	637	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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	637/637 (100%)	-0.07	5 (0%) 87 87	5, 9, 17, 24	0
1	B	637/637 (100%)	-0.09	4 (0%) 90 90	5, 9, 16, 21	0
All	All	1274/1274 (100%)	-0.08	9 (0%) 89 89	5, 9, 17, 24	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	484	LEU	3.5
1	A	177	PRO	3.3
1	B	177	PRO	3.2
1	B	530	PRO	2.8
1	A	178	GLY	2.7
1	B	252	ALA	2.6
1	A	619	GLN	2.5
1	A	620	ASN	2.4
1	B	564	THR	2.3

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	CA	B	2004	1/1	1.00	0.08	-0.32	7,7,7,7	0
2	CA	A	2001	1/1	1.00	0.08	-0.34	7,7,7,7	0
2	CA	A	2003	1/1	0.99	0.04	-2.10	12,12,12,12	0
2	CA	B	2005	1/1	1.00	0.06	-2.13	10,10,10,10	0
2	CA	B	2006	1/1	1.00	0.03	-2.32	9,9,9,9	0
2	CA	A	2002	1/1	0.98	0.06	-2.60	12,12,12,12	0

6.5 Other polymers

There are no such residues in this entry.