



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2021 – 06:00 AM EDT

PDB ID : 1MS5
Title : Triclinic form of Trypanosoma cruzi trans-sialidase, soaked with N-acetylneuraminyl- α -2,3-thio-galactoside (NA-S-Gal)
Authors : Buschiazzo, A.; Amaya, M.F.; Cremona, M.L.; Frasch, A.C.; Alzari, P.M.
Deposited on : 2002-09-19
Resolution : 2.00 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
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

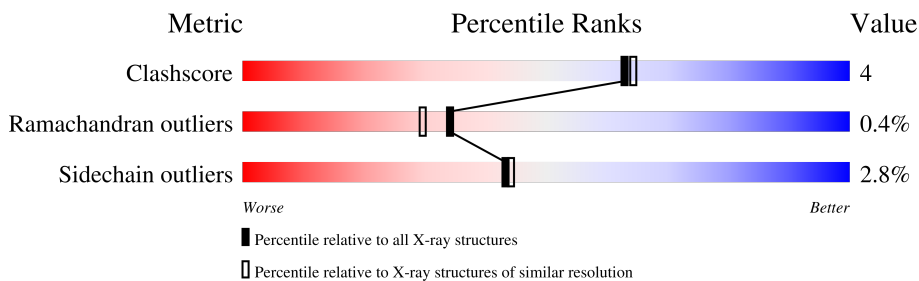
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	648	
1	B	648	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 10373 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 trans-sialidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	623	4889	3094	851	928	16	0	8	0
1	B	621	4866	3080	849	922	15	0	7	0

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	expression tag	UNP Q26964
A	-12	GLY	-	expression tag	UNP Q26964
A	-11	GLY	-	expression tag	UNP Q26964
A	-10	SER	-	expression tag	UNP Q26964
A	-9	HIS	-	expression tag	UNP Q26964
A	-8	HIS	-	expression tag	UNP Q26964
A	-7	HIS	-	expression tag	UNP Q26964
A	-6	HIS	-	expression tag	UNP Q26964
A	-5	HIS	-	expression tag	UNP Q26964
A	-4	HIS	-	expression tag	UNP Q26964
A	-3	GLY	-	expression tag	UNP Q26964
A	-2	MET	-	expression tag	UNP Q26964
A	-1	ALA	-	expression tag	UNP Q26964
A	0	SER	-	expression tag	UNP Q26964
A	58	PHE	ASN	engineered mutation	UNP Q26964
A	262	THR	SER	SEE REMARK 999	UNP Q26964
A	476	PHE	ARG	SEE REMARK 999	UNP Q26964
A	484	LEU	VAL	SEE REMARK 999	UNP Q26964
A	495	LYS	SER	engineered mutation	UNP Q26964
A	496	GLY	VAL	engineered mutation	UNP Q26964
A	520	LYS	GLU	engineered mutation	UNP Q26964
A	558	VAL	GLU	SEE REMARK 999	UNP Q26964
A	593	GLY	ASP	engineered mutation	UNP Q26964
A	597	ASP	ILE	engineered mutation	UNP Q26964
A	599	ARG	HIS	engineered mutation	UNP Q26964

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	MET	-	expression tag	UNP Q26964
B	-12	GLY	-	expression tag	UNP Q26964
B	-11	GLY	-	expression tag	UNP Q26964
B	-10	SER	-	expression tag	UNP Q26964
B	-9	HIS	-	expression tag	UNP Q26964
B	-8	HIS	-	expression tag	UNP Q26964
B	-7	HIS	-	expression tag	UNP Q26964
B	-6	HIS	-	expression tag	UNP Q26964
B	-5	HIS	-	expression tag	UNP Q26964
B	-4	HIS	-	expression tag	UNP Q26964
B	-3	GLY	-	expression tag	UNP Q26964
B	-2	MET	-	expression tag	UNP Q26964
B	-1	ALA	-	expression tag	UNP Q26964
B	0	SER	-	expression tag	UNP Q26964
B	58	PHE	ASN	engineered mutation	UNP Q26964
B	262	THR	SER	SEE REMARK 999	UNP Q26964
B	476	PHE	ARG	SEE REMARK 999	UNP Q26964
B	484	LEU	VAL	SEE REMARK 999	UNP Q26964
B	495	LYS	SER	engineered mutation	UNP Q26964
B	496	GLY	VAL	engineered mutation	UNP Q26964
B	520	LYS	GLU	engineered mutation	UNP Q26964
B	558	VAL	GLU	SEE REMARK 999	UNP Q26964
B	593	GLY	ASP	engineered mutation	UNP Q26964
B	597	ASP	ILE	engineered mutation	UNP Q26964
B	599	ARG	HIS	engineered mutation	UNP Q26964

- Molecule 2 is water.


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	279	Total O 279 279	0	0
2	B	339	Total O 339 339	0	0

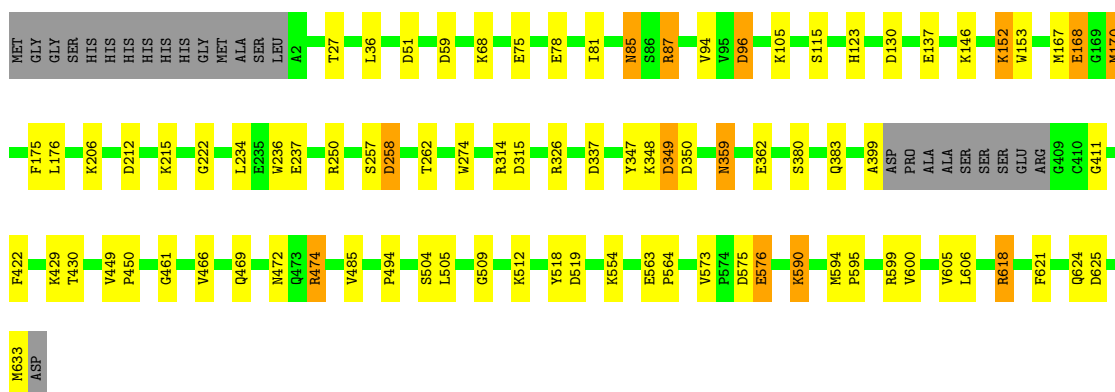
3 Residue-property plots [i](#)

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. 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. 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.


Note EDS was not executed.

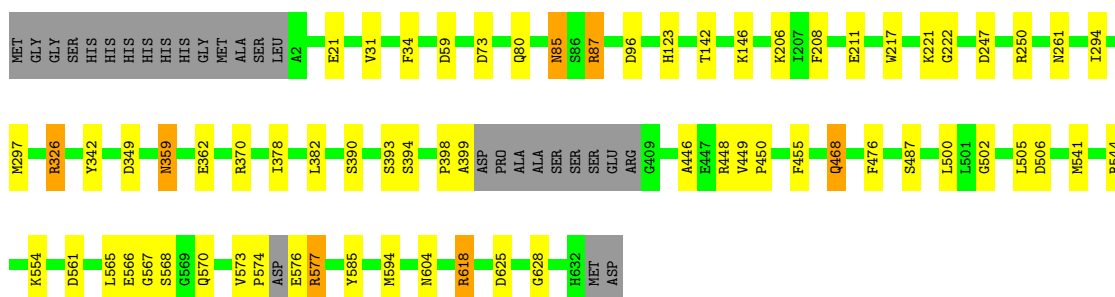
- Molecule 1: trans-sialidase

Chain A:  83% 11% . .



- Molecule 1: trans-sialidase

Chain B:  85% 9% . .



4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	51.37Å 74.69Å 88.07Å 86.00° 84.20° 88.38°	Depositor
Resolution (Å)	27.42 – 2.00	Depositor
% Data completeness (in resolution range)	73.9 (27.42-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.03	Depositor
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.170 , 0.237	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	10373	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

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	0.92	0/5003	0.96	15/6794 (0.2%)
1	B	1.01	4/4977 (0.1%)	0.99	13/6754 (0.2%)
All	All	0.96	4/9980 (0.0%)	0.97	28/13548 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	476	PHE	CE1-CZ	-5.64	1.26	1.37
1	B	21	GLU	CD-OE1	5.27	1.31	1.25
1	B	476	PHE	CD1-CE1	-5.22	1.28	1.39
1	B	476	PHE	CG-CD2	-5.12	1.31	1.38

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	250	ARG	NE-CZ-NH2	-10.28	115.16	120.30
1	A	250	ARG	NE-CZ-NH2	-9.12	115.74	120.30
1	B	250	ARG	NE-CZ-NH1	9.08	124.84	120.30
1	A	59	ASP	CB-CG-OD2	8.78	126.20	118.30
1	A	96	ASP	CB-CG-OD2	8.07	125.56	118.30
1	B	96	ASP	CB-CG-OD2	8.04	125.53	118.30
1	B	349	ASP	CB-CG-OD2	7.73	125.26	118.30
1	B	247	ASP	CB-CG-OD2	7.69	125.22	118.30
1	B	561	ASP	CB-CG-OD2	7.40	124.96	118.30
1	B	73	ASP	CB-CG-OD2	6.78	124.40	118.30
1	B	59	ASP	CB-CG-OD2	6.71	124.34	118.30
1	A	258	ASP	CB-CG-OD2	6.66	124.30	118.30
1	A	130	ASP	CB-CG-OD1	6.31	123.98	118.30
1	A	51	ASP	CB-CA-C	-6.08	98.25	110.40
1	A	314	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	A	250	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	A	337	ASP	CB-CG-OD2	5.87	123.58	118.30
1	B	326	ARG	NE-CZ-NH1	5.75	123.17	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	506	ASP	CB-CG-OD1	5.71	123.44	118.30
1	A	87	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	A	349	ASP	CB-CG-OD2	5.68	123.41	118.30
1	B	370	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	A	625	ASP	CB-CG-OD2	5.48	123.23	118.30
1	A	212	ASP	CB-CG-OD2	5.43	123.19	118.30
1	B	326	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	A	315	ASP	CB-CG-OD2	5.32	123.09	118.30
1	B	448	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	A	87	ARG	CG-CD-NE	5.04	122.39	111.80

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	4889	0	4783	49	0
1	B	4866	0	4781	34	0
2	A	279	0	0	2	0
2	B	339	0	0	3	0
All	All	10373	0	9564	83	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 4.

All (83) 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:380:SER:O	1:A:383[B]:GLN:HG3	1.71	0.91
1:A:509:GLY:O	1:A:512:LYS:NZ	2.03	0.90
1:B:576:GLU:O	1:B:577:ARG:CB	2.21	0.86
1:B:85:ASN:HD22	1:B:87:ARG:H	1.27	0.81
1:A:618:ARG:HG2	1:A:618:ARG:HH11	1.49	0.77
1:B:221[B]:LYS:HA	1:B:221[B]:LYS:HE2	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:ASN:HD22	1:A:87:ARG:H	1.34	0.73
1:A:469:GLN:OE1	1:A:474:ARG:HD3	1.90	0.72
1:A:359:ASN:HD21	1:A:362:GLU:H	1.38	0.72
1:B:359:ASN:HD21	1:B:362:GLU:H	1.41	0.68
1:A:170:MET:HG2	2:A:775:HOH:O	1.93	0.66
1:B:554:LYS:HB3	1:B:573:VAL:HG13	1.78	0.65
1:B:221[B]:LYS:HA	1:B:221[B]:LYS:CE	2.27	0.64
1:B:85:ASN:ND2	1:B:87:ARG:H	1.96	0.63
1:A:85:ASN:ND2	1:A:87:ARG:H	1.98	0.61
1:A:422:PHE:CD2	1:A:606:LEU:HD23	2.36	0.60
1:B:565:LEU:O	1:B:566:GLU:C	2.40	0.60
1:B:487:SER:HB3	1:B:544:ARG:HE	1.64	0.60
1:A:554:LYS:HG2	1:A:573:VAL:HG13	1.84	0.60
1:A:36:LEU:HD23	1:A:96:ASP:HA	1.83	0.59
1:A:618:ARG:HG2	1:A:618:ARG:NH1	2.16	0.58
1:B:398:PRO:O	1:B:399:ALA:CB	2.52	0.58
1:A:449:VAL:HB	1:A:450:PRO:CD	2.33	0.57
1:B:206:LYS:NZ	2:B:769:HOH:O	2.36	0.57
1:A:27:THR:HG23	2:A:911:HOH:O	2.07	0.55
1:A:494:PRO:HG3	1:A:518:TYR:CE1	2.43	0.54
1:B:594:MET:CE	1:B:594:MET:HA	2.37	0.54
1:B:567:GLY:O	1:B:570:GLN:NE2	2.40	0.53
1:A:152:LYS:HD3	1:A:153:TRP:N	2.25	0.52
1:A:105:LYS:HZ2	1:A:137:GLU:CD	2.13	0.51
1:A:152:LYS:HD3	1:A:152:LYS:C	2.31	0.51
1:A:167:MET:O	1:A:168:GLU:C	2.50	0.50
1:B:618[A]:ARG:HH11	1:B:618[A]:ARG:HG2	1.76	0.50
1:B:294:ILE:O	1:B:297[B]:MET:HG3	2.11	0.50
1:A:399:ALA:HB2	1:A:411:GLY:CA	2.42	0.50
1:B:554:LYS:CB	1:B:573:VAL:HG13	2.41	0.49
1:A:380:SER:HA	1:A:383[B]:GLN:CG	2.43	0.49
1:B:221[B]:LYS:CE	1:B:221[B]:LYS:CA	2.90	0.49
1:A:234:LEU:C	1:A:234:LEU:HD12	2.35	0.47
1:A:380:SER:C	1:A:383[B]:GLN:HG3	2.35	0.47
1:B:502:GLY:HA3	1:B:585:TYR:CZ	2.49	0.47
1:A:359:ASN:HD21	1:A:362:GLU:N	2.08	0.47
1:B:142:THR:HA	1:B:146:LYS:O	2.14	0.47
1:A:554:LYS:CG	1:A:573:VAL:HG13	2.44	0.47
1:A:554:LYS:HG2	1:A:573:VAL:CG1	2.45	0.46
1:A:105:LYS:NZ	1:A:137:GLU:OE2	2.44	0.46
1:A:236:TRP:CD1	1:A:237:GLU:HG3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:359:ASN:HD21	1:B:362:GLU:N	2.12	0.46
1:A:594:MET:HA	1:A:595:PRO:HD3	1.84	0.46
1:B:206:LYS:HE2	1:B:222:GLY:O	2.16	0.45
1:A:258:ASP:OD2	1:A:262:THR:OG1	2.29	0.45
1:A:347:TYR:CE1	1:A:350:ASP:HA	2.52	0.45
1:A:519:ASP:OD1	1:A:519:ASP:C	2.56	0.44
1:A:485:VAL:O	1:A:605:VAL:HA	2.17	0.44
1:A:68:LYS:HA	1:A:78:GLU:O	2.17	0.44
1:B:208:PHE:CE2	1:B:217:TRP:HB3	2.53	0.44
1:A:206:LYS:HD2	1:A:222:GLY:O	2.17	0.43
1:A:348:LYS:HE3	1:A:349:ASP:OD2	2.19	0.43
1:A:215:LYS:HD3	1:A:215:LYS:HA	1.80	0.43
1:A:599:ARG:C	1:A:600:VAL:HG13	2.39	0.43
1:B:85:ASN:HD22	1:B:85:ASN:C	2.22	0.42
1:A:429:LYS:HE3	1:A:430:THR:HG23	2.00	0.42
1:A:461:GLY:O	1:A:590:LYS:HG3	2.18	0.42
1:B:390:SER:O	1:B:394:SER:HB3	2.18	0.42
1:B:211:GLU:OE1	2:B:844:HOH:O	2.21	0.42
1:B:221[A]:LYS:HG3	1:B:261:ASN:OD1	2.20	0.42
1:B:449:VAL:HB	1:B:450:PRO:HD2	2.02	0.42
1:A:81:ILE:HD13	1:A:81:ILE:HA	1.90	0.42
1:B:378:ILE:O	1:B:382:LEU:HG	2.19	0.42
1:B:446:ALA:HB2	1:B:455:PHE:CE2	2.55	0.41
1:B:573:VAL:HA	1:B:574:PRO:HD3	1.93	0.41
1:B:604:ASN:HD21	1:B:628:GLY:HA2	1.85	0.41
1:A:175:PHE:O	1:A:176:LEU:HD23	2.20	0.41
1:A:504:SER:OG	1:A:509:GLY:HA2	2.21	0.41
1:A:168:GLU:CD	1:A:168:GLU:N	2.74	0.41
1:A:274:TRP:HA	1:A:472:ASN:HD22	1.86	0.41
1:A:563:GLU:HA	1:A:564:PRO:HD3	1.95	0.41
1:A:621:PHE:O	1:A:624:GLN:HG3	2.21	0.41
1:A:494:PRO:HG3	1:A:518:TYR:CD1	2.57	0.40
1:A:575:ASP:O	1:A:576:GLU:CB	2.69	0.40
1:B:31:VAL:HB	1:B:34:PHE:CZ	2.56	0.40
1:B:342:TYR:CD1	1:B:342:TYR:N	2.88	0.40
1:B:468:GLN:NE2	2:B:862:HOH:O	2.44	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	627/648 (97%)	603 (96%)	21 (3%)	3 (0%)	29	23
1	B	622/648 (96%)	596 (96%)	24 (4%)	2 (0%)	41	37
All	All	1249/1296 (96%)	1199 (96%)	45 (4%)	5 (0%)	34	30

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	577	ARG
1	A	168	GLU
1	A	576	GLU
1	B	468	GLN
1	A	466	VAL

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	531/547 (97%)	514 (97%)	17 (3%)	39	38
1	B	529/547 (97%)	515 (97%)	14 (3%)	46	48
All	All	1060/1094 (97%)	1029 (97%)	31 (3%)	43	43

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	GLU

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Mol	Chain	Res	Type
1	A	85	ASN
1	A	94	VAL
1	A	115[A]	SER
1	A	115[B]	SER
1	A	123	HIS
1	A	146	LYS
1	A	152	LYS
1	A	170	MET
1	A	257	SER
1	A	326	ARG
1	A	359	ASN
1	A	474	ARG
1	A	505	LEU
1	A	590	LYS
1	A	618	ARG
1	A	633	MET
1	B	80	GLN
1	B	85	ASN
1	B	87	ARG
1	B	123	HIS
1	B	326	ARG
1	B	359	ASN
1	B	393	SER
1	B	500	LEU
1	B	505	LEU
1	B	541	MET
1	B	568	SER
1	B	618[A]	ARG
1	B	618[B]	ARG
1	B	625	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	ASN
1	A	123	HIS
1	A	174	GLN
1	A	359	ASN
1	A	468	GLN
1	A	472	ASN
1	A	553	ASN
1	A	603	ASN

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Mol	Chain	Res	Type
1	A	604	ASN
1	B	85	ASN
1	B	123	HIS
1	B	174	GLN
1	B	359	ASN
1	B	468	GLN
1	B	604	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 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 [i](#)

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.