wwPDB X-ray Structure Validation Summary Report (i)

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PDB ID	:	1M7X
Title	:	The X-ray Crystallographic Structure of Branching Enzyme
Authors	:	Abad, M.C.; Binderup, K.; Rios-Steiner, J.; Arni, R.K.; Preiss, J.; Geiger, J.H.
Deposited on	:	2002-07-23
Resolution	:	2.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

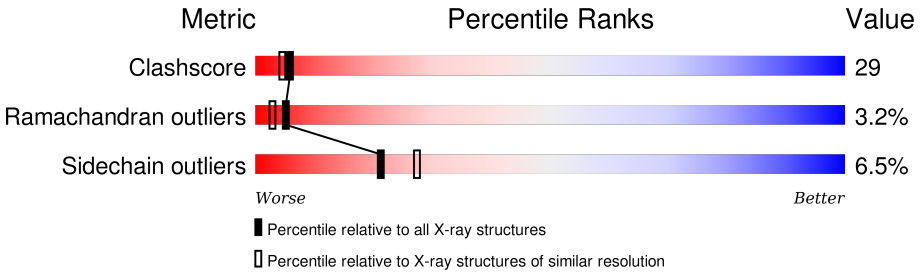
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)

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 <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	617	51% 37% 7% 5%
1	B	617	54% 35% 7% .
1	C	617	42% 45% 6% 6%
1	D	617	53% 37% 5% 5%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 20372 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 1,4-alpha-glucan Branching Enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	587	Total	C	N	O	S	0	0	0
			4823	3083	857	867	16			
1	B	591	Total	C	N	O	S	0	0	0
			4852	3102	859	876	15			
1	C	578	Total	C	N	O	S	0	0	0
			4750	3041	840	854	15			
1	D	585	Total	C	N	O	S	0	0	0
			4805	3072	853	864	16			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	112	MET	-	INITIATING MET	UNP P07762
B	112	MET	-	INITIATING MET	UNP P07762
C	112	MET	-	INITIATING MET	UNP P07762
D	112	MET	-	INITIATING MET	UNP P07762

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	301	Total	O	0	0
			301	301		
2	B	425	Total	O	0	0
			425	425		
2	C	108	Total	O	0	0
			108	108		
2	D	308	Total	O	0	0
			308	308		

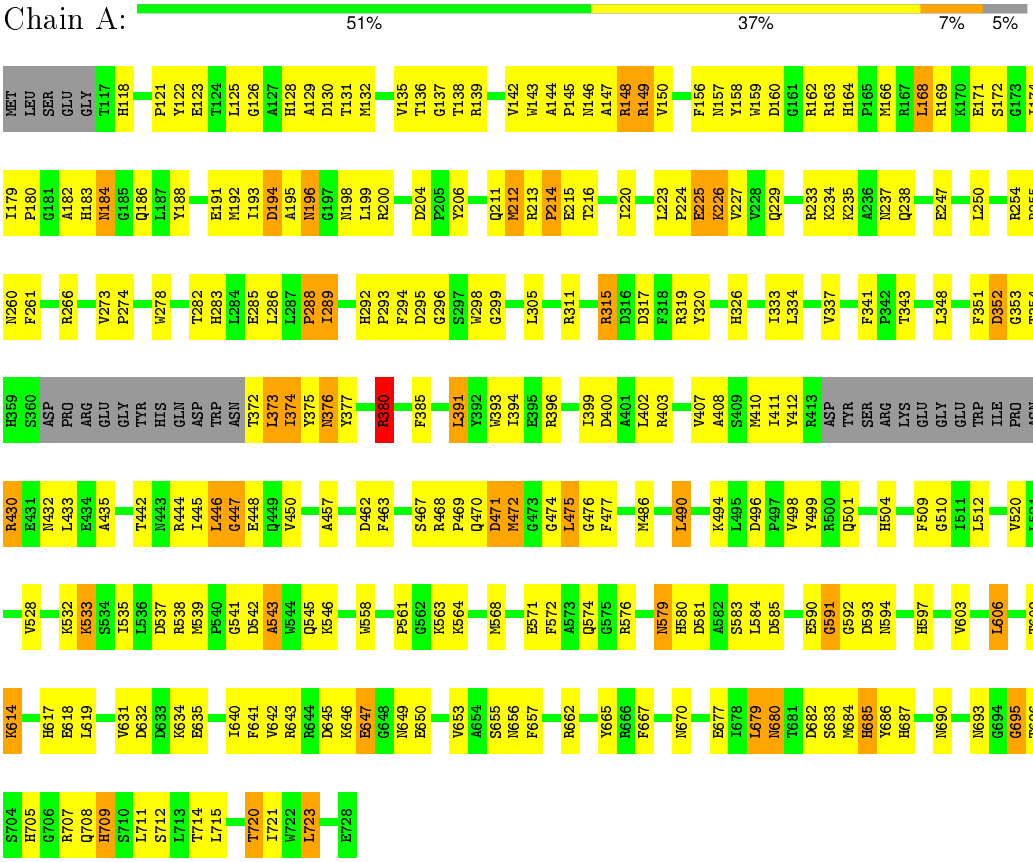
3 Residue-property plots (i)

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.

Note EDS was not executed.

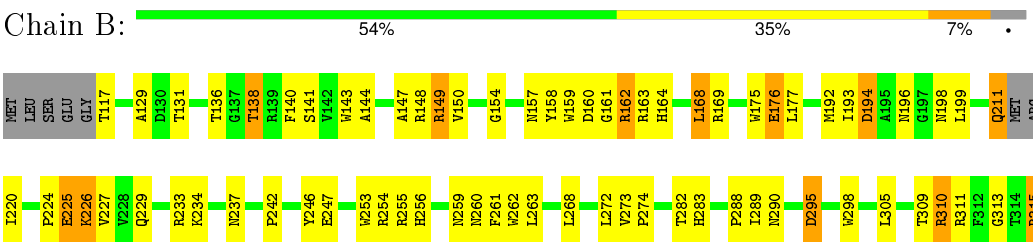
- Molecule 1: 1,4-alpha-glucan Branching Enzyme

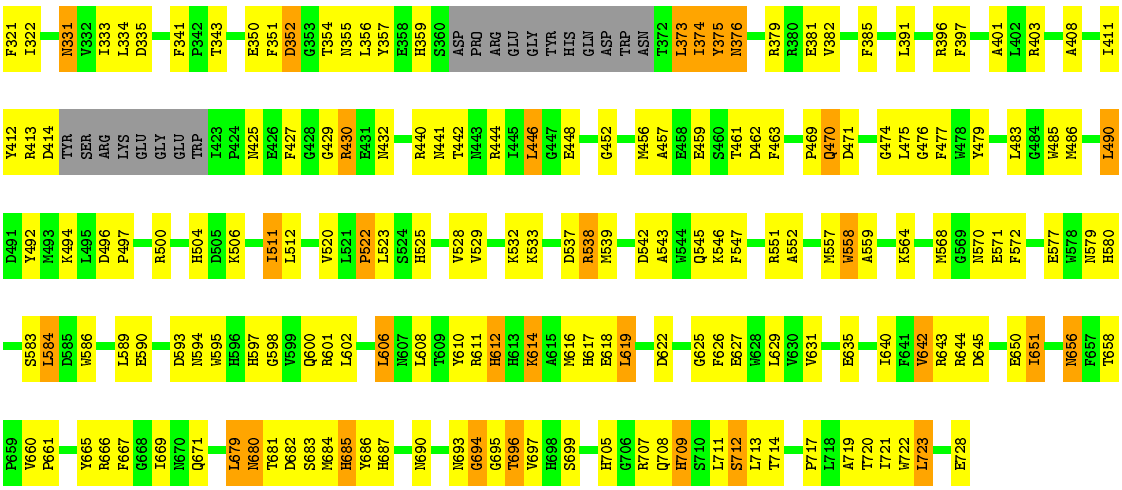
Chain A:



- Molecule 1: 1,4-alpha-glucan Branching Enzyme

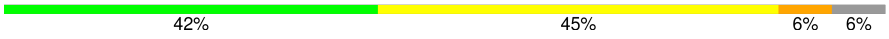
Chain B:

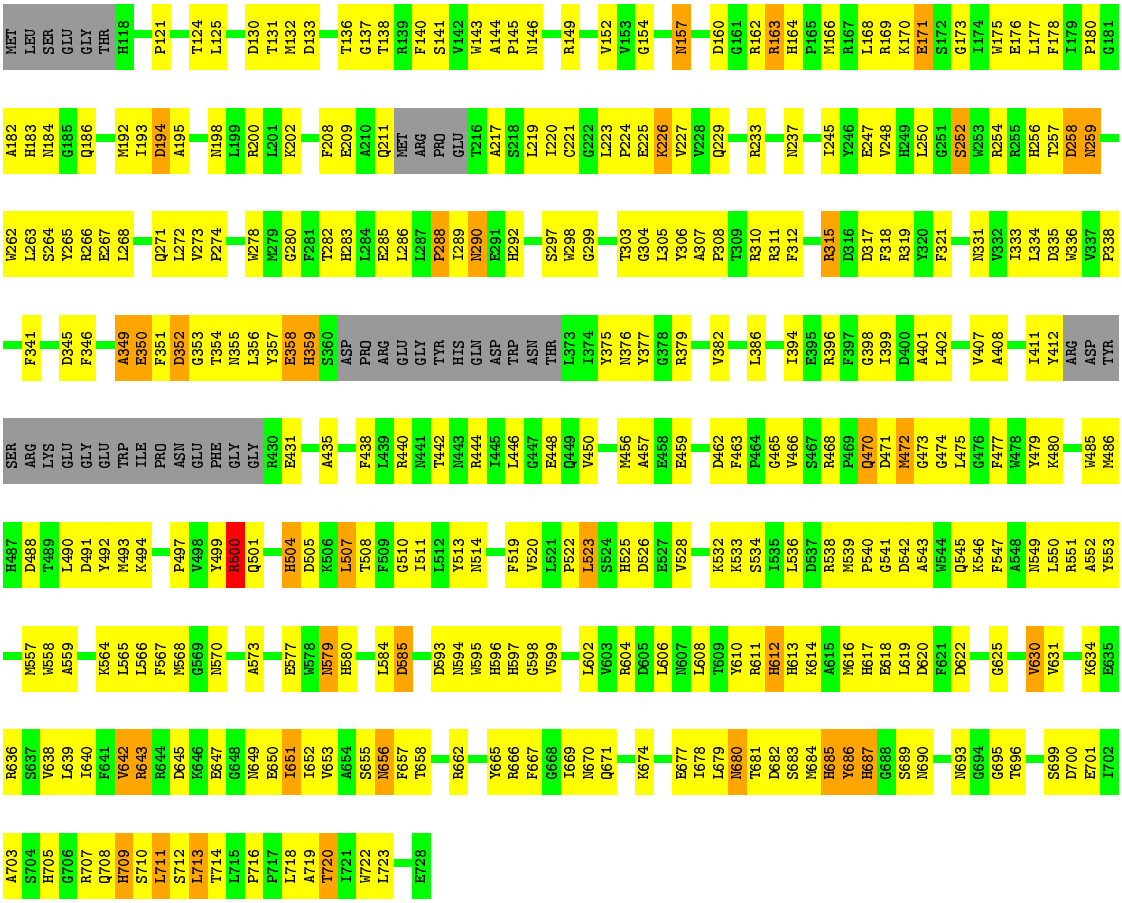




• Molecule 1: 1,4-alpha-glucan Branching Enzyme

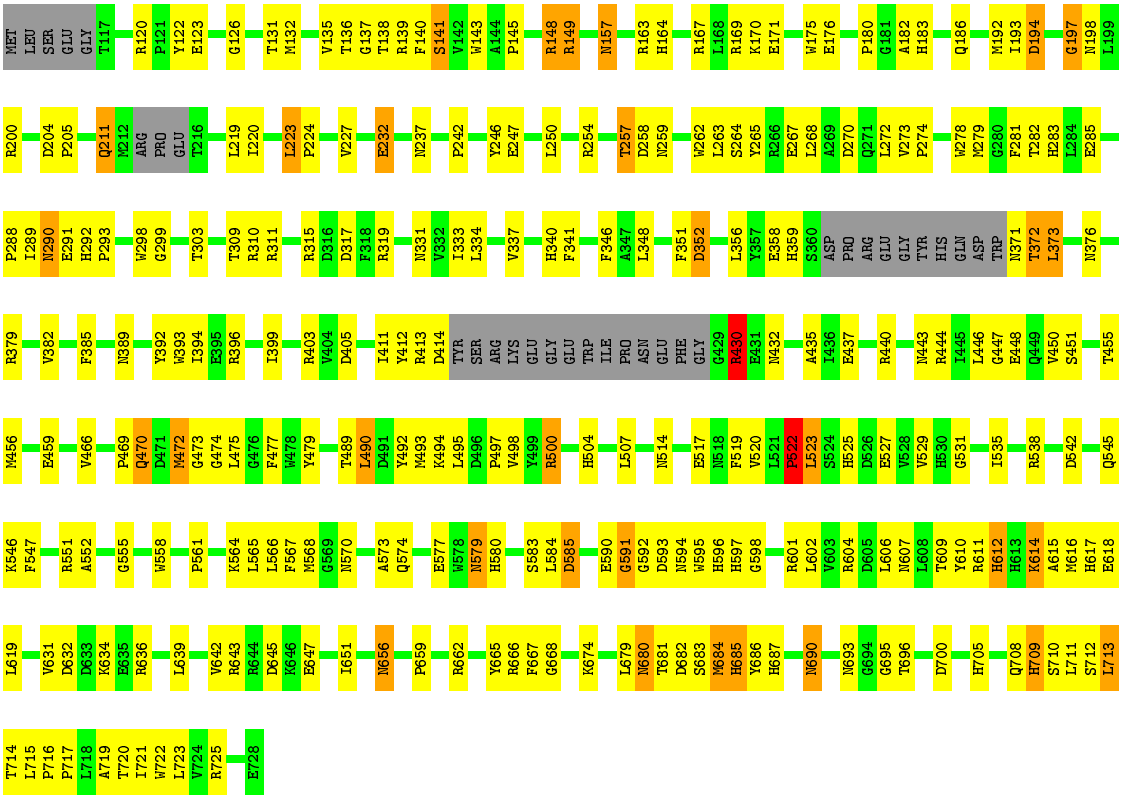
Chain C:





• Molecule 1: 1,4-alpha-glucan Branching Enzyme

Chain D:


MET R120 G126 T131 V135 R148 N157 R163 R167 P180 M192 G197
LEU P121 M132 T136 R149 H164 L168 G181 I193 N198
SER Y122 G137 R169 A182 D194 L199
GLU E123 T138 K170 H183
GLY T117 R139 E171 Q186
F140 W175
S141 E176
R200 D204 P205 Q211 M212 T216 L219 I220 L223 P224 V227 E232 N237 P242 Y246 E247 L250 R254 T257 D258 N259 W262 L263 S264 Y265 R266 E267 L268 A269 D270 Q271 L272 V273 P274 W278 M279 G280 F281 T282 H283 L284 E285
ARG
PRO
GLU
P288 I289 N290 E291 H292 P293 W298 G299 T303 T309 R310 R311 R315 D316 D317 F318 R319 N331 V332 I333 L334 V337 H340 F341 F346 A347 L348 F351 D352 L356 Y357 E358 H359 S360 N371 T372 L373 N376
ASP
PRO
ARG
GLU
GLY
TYR
HIS
GLN
ASP
TRP
R379 V382 F385 N389 Y392 W393 I394 E395 R396 I399 R403 V404 D405 I411 Y412 R413 D414 G429 R430 E431 N432 A435 I436 E437 R440 N443 R444 I445 L446 G447 E448 Q449 V450 S451 T455
TYR
SER
ARG
LYS
GLU
GLY
GLU
TRP
ILE
PRO
ASN
GLU
PHE
GLY
M456 E459 V466 P469 Q470 D471 M472 G473 G474 L475 G476 F477 W478 Y479 T489 L490 D491 Y492 M493 K494 L495 D496 P497 V498 Y499 R500 H504 L507 N514 E517 N518 F519 V520 L521 P522 L523 S524 H525 D526 E527 V528 V529 H530 G531 I535 R538 D542 Q545
K546 F547 R551 A552 G555 W558 P561 K564 L565 L566 F567 M568 G569 N570 A573 Q574 E577 W578 N579 H580 S583 L584 D585 E590 G591 G592 D593 N594 W595 H596 H597 G598 R601 L602 V603 R604 D605 L606 N607 L608 T609 Y610 R611 H612 H613 K614 A615 H616 H617 E618
L619 V631 D632 D633 K634 E635 R636 L639 V642 R643 R644 D645 K646 E647 I651 N656 P659 R662 Y665 R666 F667 G668 K674 L679 N680 T681 D682 S683 M684 H685 Y686 H687 N690 N693 G694 G695 T696 D700 H705 Q708 H709 S710 L711 S712 L713
T714 L715 P716 P717 L718 A719 T720 I721 W722 L723 V724 R725 E728

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	91.47Å 102.62Å 185.06Å 90.00° 91.45° 90.00°	Depositor
Resolution (Å)	35.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (35.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.200 , 0.265	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	20372	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

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	0/4976	0.68	1/6756 (0.0%)
1	B	0.42	0/5006	0.70	2/6797 (0.0%)
1	C	0.39	0/4900	0.61	0/6653
1	D	0.42	0/4956	0.69	1/6728 (0.0%)
All	All	0.41	0/19838	0.67	4/26934 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	375	TYR	N-CA-C	6.06	127.35	111.00
1	A	685	HIS	N-CA-C	-5.83	95.25	111.00
1	B	685	HIS	N-CA-C	-5.75	95.46	111.00
1	D	685	HIS	N-CA-C	-5.36	96.53	111.00

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	4823	0	4559	263	0
1	B	4852	0	4571	255	0
1	C	4750	0	4485	325	0
1	D	4805	0	4537	240	0
2	A	301	0	0	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	425	0	0	33	0
2	C	108	0	0	21	0
2	D	308	0	0	20	0
All	All	20372	0	18152	1077	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 29.

The worst 5 of 1077 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:C:643:ARG:HB3	1:C:643:ARG:HH11	1.12	1.08
1:C:497:PRO:HA	1:C:500:ARG:HD3	1.42	1.02
1:A:430:ARG:HH21	1:A:430:ARG:HB3	1.22	1.02
1:A:224:PRO:HG2	1:A:396:ARG:HB3	1.38	1.01
1:B:430:ARG:H	1:B:430:ARG:HD2	1.22	1.01

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	581/617 (94%)	502 (86%)	52 (9%)	27 (5%)	3 1
1	B	583/617 (94%)	522 (90%)	48 (8%)	13 (2%)	8 6
1	C	570/617 (92%)	494 (87%)	57 (10%)	19 (3%)	5 3
1	D	577/617 (94%)	522 (90%)	40 (7%)	15 (3%)	7 4
All	All	2311/2468 (94%)	2040 (88%)	197 (8%)	74 (3%)	5 3

5 of 74 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	148	ARG
1	A	212	MET
1	A	215	GLU
1	A	225	GLU
1	A	257	THR

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	498/525 (95%)	466 (94%)	32 (6%)	22	28
1	B	501/525 (95%)	464 (93%)	37 (7%)	17	21
1	C	490/525 (93%)	460 (94%)	30 (6%)	23	30
1	D	496/525 (94%)	466 (94%)	30 (6%)	24	31
All	All	1985/2100 (94%)	1856 (94%)	129 (6%)	21	27

5 of 129 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	558	TRP
1	C	163	ARG
1	D	579	ASN
1	B	606	LEU
1	B	656	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 121 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	656	ASN
1	C	256	HIS
1	D	617	HIS
1	B	687	HIS
1	C	146	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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.