



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 10:08 PM UTC

PDB ID : 1WE0 / pdb_00001we0
Title : Crystal structure of peroxiredoxin (AhpC) from *Amphibacillus xylanus*
Authors : Kitano, K.; Kita, A.; Hakoshima, T.; Niimura, Y.; Miki, K.
Deposited on : 2004-05-21
Resolution : 2.90 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

<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
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

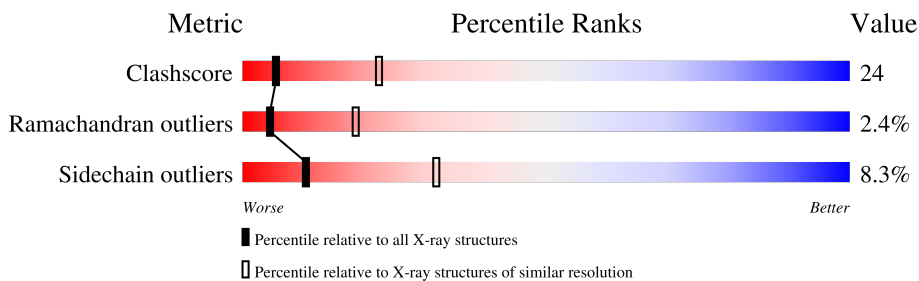
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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))
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)



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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	187	
1	B	187	
1	C	187	
1	D	187	
1	E	187	
1	F	187	
1	G	187	
1	H	187	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain				
1	I	187		52%	31%	6%	11%
1	J	187		48%	34%	7%	11%

2 Entry composition [i](#)

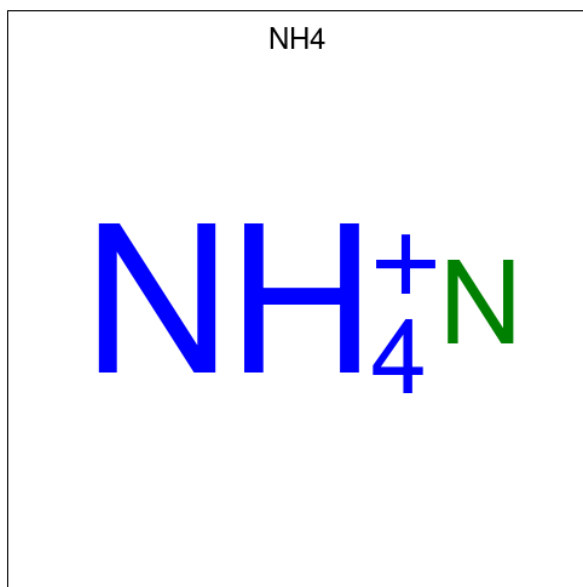
There are 2 unique types of molecules in this entry. The entry contains 12982 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 alkyl hydroperoxide reductase C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	166	1298	826	211	258	3	0	0	0
1	B	166	1298	826	211	258	3	0	0	0
1	C	166	1298	826	211	258	3	0	0	0
1	D	166	1298	826	211	258	3	0	0	0
1	E	166	1298	826	211	258	3	0	0	0
1	F	166	1298	826	211	258	3	0	0	0
1	G	166	1298	826	211	258	3	0	0	0
1	H	166	1298	826	211	258	3	0	0	0
1	I	166	1298	826	211	258	3	0	0	0
1	J	166	1298	826	211	258	3	0	0	0

- Molecule 2 is AMMONIUM ION (CCD ID: NH4) (formula: H₄N).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	F	1	Total N 1 1	0	0
2	J	1	Total N 1 1	0	0

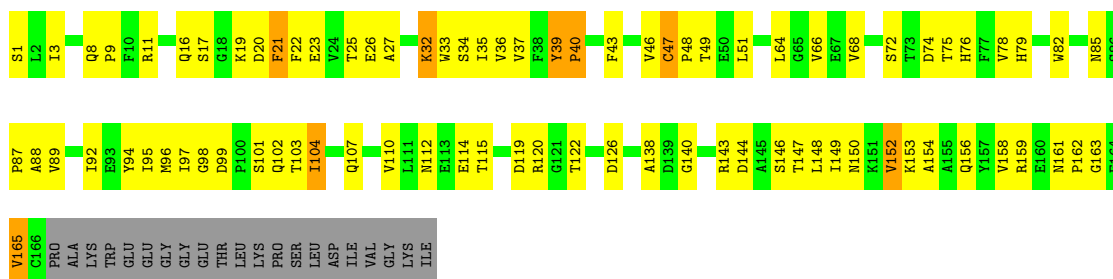
3 Residue-property plots

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. 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.

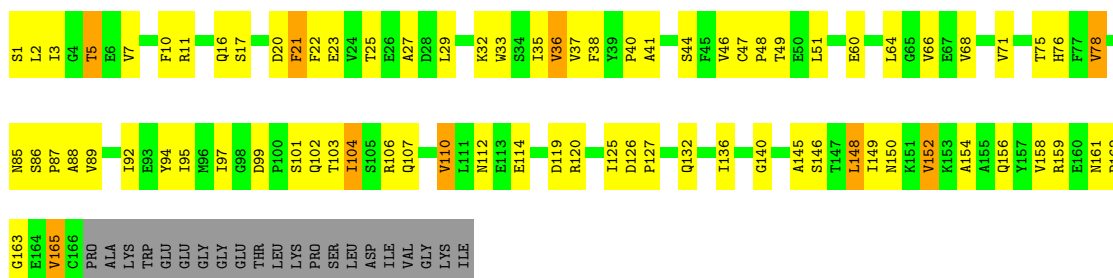
- Molecule 1: alkyl hydroperoxide reductase C

Chain A: 



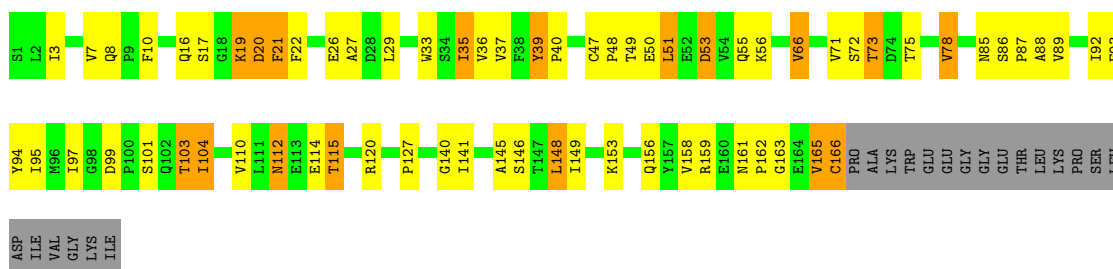
- Molecule 1: alkyl hydroperoxide reductase C

Chain B: 



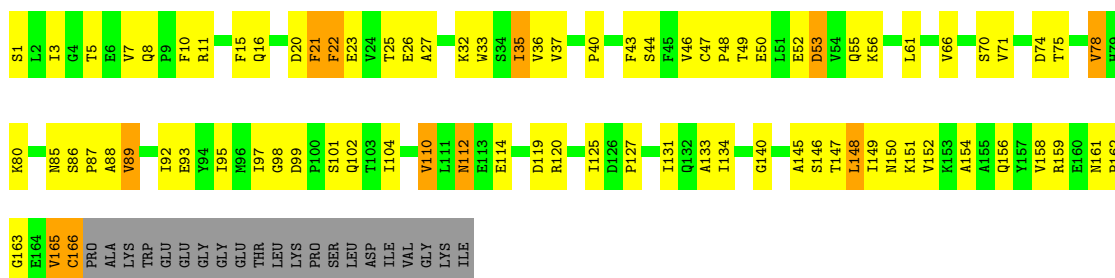
- Molecule 1: alkyl hydroperoxide reductase C

Chain C: 



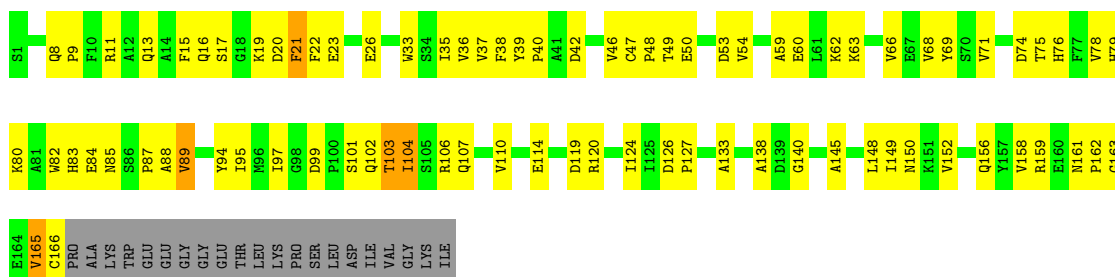
- Molecule 1: alkyl hydroperoxide reductase C

Chain D:  44% 39% 6% 11%



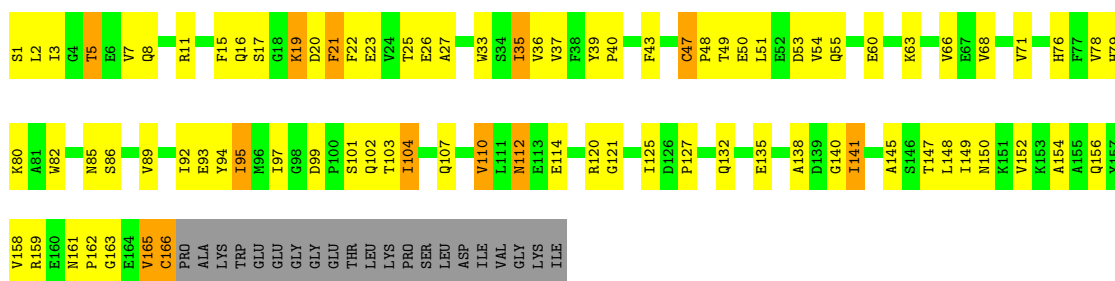
- Molecule 1: alkyl hydroperoxide reductase C

Chain E:  45% 41% 11%



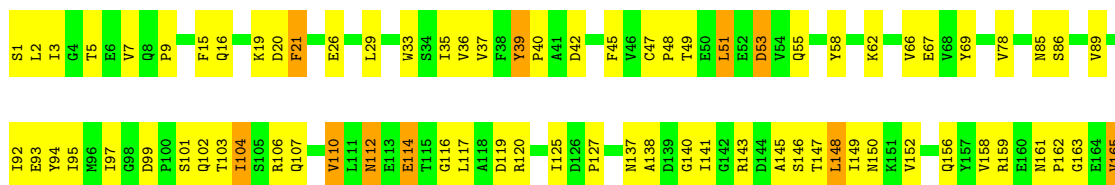
- Molecule 1: alkyl hydroperoxide reductase C

Chain F:  44% 39% 6% 11%



- Molecule 1: alkyl hydroperoxide reductase C

Chain G:  48% 36% 5% 11%



C166
 PRO
 ALA
 LYS
 LYS
 TRP
 GLU
 TRP
 GLU
 GLU
 GLY
 GLY
 THR
 THR
 LEU
 LEU
 LYS
 LYS
 PRO
 PRO
 SER
 LEU
 SER
 ASP
 ILE
 ILE
 VAL
 VAL
 GLY
 LYS
 ILE

- Molecule 1: alkyl hydroperoxide reductase C

Chain H: 44% 37% 7% 11%

S1 L2 L3 Q8 P9 F10 R11 Q16 K19 D20 F21 E26 K32 W33 S34 I35 V36 V37 F38 V39 P40 F43 V46 C47 P48 T49 E50 L51 E52 D53 V54 Q55 K56 E57 Y58 L61 K62 V66 E67 V68 Y69 S70 V71 V78 H79 K80 E84 N85 S86

P87 A88 W89 I92 Q93 Y94 I95 I96 I97 S101 O102 T103 S106 R106 Q107 V110 L111 N112 E113 I114 T115 D119 R120 T124 I125 D126 P127 I131 Q132 E133 A133 G140 A145 S146 T147 L148 V152 K153 A154 A155 Q156 Y157 V158 R159 E160 N161 P162 G163 E164 V165 C166

PRO
 ALA
 LYS
 TRP
 GLU
 TRP
 GLU
 GLY
 GLY
 THR
 THR
 LEU
 LYS
 PRO
 PRO
 SER
 LEU
 ASP
 ILE
 VAL
 VAL
 GLY
 LYS
 ILE

- Molecule 1: alkyl hydroperoxide reductase C

Chain I: 52% 31% 6% 11%

S1 L2 I3 Q8 P9 F10 R11 K19 D20 F21 E22 E23 V24 T25 E26 A27 D28 W33 S34 I35 V36 V37 P40 C47 P48 T49 E52 D53 V54 Q55 Y58 K62 V66 V71 D74 T75 H76 F77 V78 N85 S86 P87 A88 V89 I92 E93 Y94

I95 I96 G98 P100 S101 Q102 T103 I104 Q107 V110 L111 N112 E113 E114 D119 R120 P127 I131 A138 D139 G140 D144 T147 L148 V152 K153 A154 A155 Y157 V158 R159 E160 M161 P162 G163 V165 C166 PRO ALA LYS TRP GLU GLY THR

LEU
 LYS
 PRO
 SER
 LEU
 ASP
 ILE
 VAL
 GLY
 LYS
 ILE

- Molecule 1: alkyl hydroperoxide reductase C

Chain J: 48% 34% 7% 11%

S1 L2 I3 T5 Q8 P9 F10 R11 Q16 K19 D20 F21 F22 G23 V24 T25 E26 A27 W33 S34 I35 V36 V37 F38 P40 F43 S44 F45 V46 C47 P48 T49 E50 L51 E52 D53 V54 Q55 L64 G65 V66 E67 V68 Y69 S70 V71 D74 T75 H76 F77 V78

H79 W82 N85 S86 P87 A88 W89 I92 E93 Y94 I95 I96 G98 D99 F100 S101 Q102 T103 I104 R106 Q107 V110 L111 N112 F113 E114 T115 R120 P127 D128 G140 A145 S146 T147 L148 I149 N150 Q156 Y157 V158 R159 E160 N161 P162 G163 E164 V165 C166 PRO

ALA
 LYS
 TRP
 GLU
 TRP
 GLU
 GLY
 GLY
 THR
 LEU
 LYS
 PRO
 PRO
 SER
 LEU
 ASP
 ILE
 VAL
 GLY
 LYS
 ILE

4 Data and refinement statistics

Xtriage (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	79.22Å 79.32Å 104.45Å 77.22° 82.33° 80.08°	Depositor
Resolution (Å)	50.00 – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) (50.00-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.208 , 0.235	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12982	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NH4

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	0.50	0/1326	0.96	7/1800 (0.4%)
1	B	0.49	0/1326	0.92	1/1800 (0.1%)
1	C	0.50	0/1326	0.94	6/1800 (0.3%)
1	D	0.45	0/1326	0.93	4/1800 (0.2%)
1	E	0.43	0/1326	0.93	4/1800 (0.2%)
1	F	0.48	0/1326	0.97	6/1800 (0.3%)
1	G	0.49	0/1326	0.95	4/1800 (0.2%)
1	H	0.46	0/1326	0.93	7/1800 (0.4%)
1	I	0.49	0/1326	0.95	5/1800 (0.3%)
1	J	0.52	1/1326 (0.1%)	0.95	3/1800 (0.2%)
All	All	0.48	1/13260 (0.0%)	0.94	47/18000 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	110	VAL	CA-CB	5.38	1.61	1.54

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	8	GLN	CA-C-N	6.29	126.63	119.83
1	E	8	GLN	C-N-CA	6.29	126.63	119.83
1	I	114	GLU	N-CA-C	6.18	118.98	111.82
1	G	114	GLU	N-CA-C	5.96	118.74	111.82
1	J	114	GLU	N-CA-C	5.92	118.68	111.82

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	1298	0	1252	65	0
1	B	1298	0	1252	62	0
1	C	1298	0	1252	58	0
1	D	1298	0	1252	74	0
1	E	1298	0	1252	58	0
1	F	1298	0	1252	68	0
1	G	1298	0	1252	63	0
1	H	1298	0	1252	74	0
1	I	1298	0	1252	59	0
1	J	1298	0	1252	74	0
2	F	1	0	0	0	0
2	J	1	0	0	0	0
All	All	12982	0	12520	606	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 24.

The worst 5 of 606 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:85:ASN:ND2	1:J:85:ASN:HD22	1.53	1.06
1:B:85:ASN:HD22	1:C:85:ASN:HD22	1.12	0.96
1:D:85:ASN:HD22	1:E:85:ASN:ND2	1.63	0.96
1:A:85:ASN:HD22	1:J:85:ASN:HD22	1.03	0.94
1:H:85:ASN:HD22	1:I:85:ASN:HD22	1.13	0.92

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	164/187 (88%)	144 (88%)	16 (10%)	4 (2%)	4	18
1	B	164/187 (88%)	143 (87%)	17 (10%)	4 (2%)	4	18
1	C	164/187 (88%)	143 (87%)	17 (10%)	4 (2%)	4	18
1	D	164/187 (88%)	143 (87%)	17 (10%)	4 (2%)	4	18
1	E	164/187 (88%)	144 (88%)	16 (10%)	4 (2%)	4	18
1	F	164/187 (88%)	145 (88%)	15 (9%)	4 (2%)	4	18
1	G	164/187 (88%)	145 (88%)	15 (9%)	4 (2%)	4	18
1	H	164/187 (88%)	144 (88%)	16 (10%)	4 (2%)	4	18
1	I	164/187 (88%)	143 (87%)	17 (10%)	4 (2%)	4	18
1	J	164/187 (88%)	143 (87%)	17 (10%)	4 (2%)	4	18
All	All	1640/1870 (88%)	1437 (88%)	163 (10%)	40 (2%)	4	18

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	21	PHE
1	B	21	PHE
1	C	21	PHE
1	D	21	PHE
1	E	21	PHE

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	141/158 (89%)	135 (96%)	6 (4%)	26	60
1	B	141/158 (89%)	131 (93%)	10 (7%)	13	40
1	C	141/158 (89%)	124 (88%)	17 (12%)	5	16
1	D	141/158 (89%)	128 (91%)	13 (9%)	8	27

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	141/158 (89%)	134 (95%)	7 (5%)	22	53
1	F	141/158 (89%)	128 (91%)	13 (9%)	8	27
1	G	141/158 (89%)	129 (92%)	12 (8%)	10	31
1	H	141/158 (89%)	126 (89%)	15 (11%)	6	22
1	I	141/158 (89%)	131 (93%)	10 (7%)	13	40
1	J	141/158 (89%)	127 (90%)	14 (10%)	7	24
All	All	1410/1580 (89%)	1293 (92%)	117 (8%)	10	32

5 of 117 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	37	VAL
1	J	103	THR
1	G	78	VAL
1	J	78	VAL
1	I	89	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 60 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	102	GLN
1	J	107	GLN
1	G	85	ASN
1	J	102	GLN
1	J	156	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are modelled with single atom - 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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.