



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:29 PM GMT

PDB ID : 1AZZ
Title : FIDDLER CRAB COLLAGENASE COMPLEXED TO ECOTIN
Authors : Perona, J.J.; Fletterick, R.J.
Deposited on : 1997-11-24
Resolution : 2.30 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) : **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

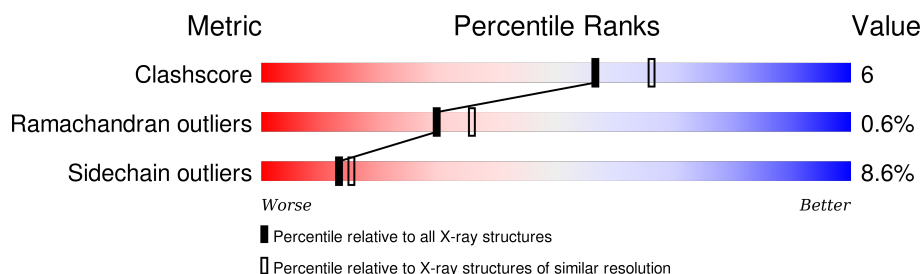
1 Overall quality at a glance

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 $\leq 5\%$. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	226	 79% 18% .
1	B	226	 76% 22% .
2	C	142	 77% 18% ..
2	D	142	 68% 26% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5527 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 COLLAGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	226	Total	C	N	O	S	0	0	0
			1653	1043	267	334	9			
1	B	226	Total	C	N	O	S	0	0	0
			1653	1043	267	334	9			

- Molecule 2 is a protein called ECOTIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	137	Total	C	N	O	S	0	0	0
			1048	671	175	196	6			
2	D	138	Total	C	N	O	S	0	0	0
			1033	661	173	193	6			

- Molecule 3 is water.

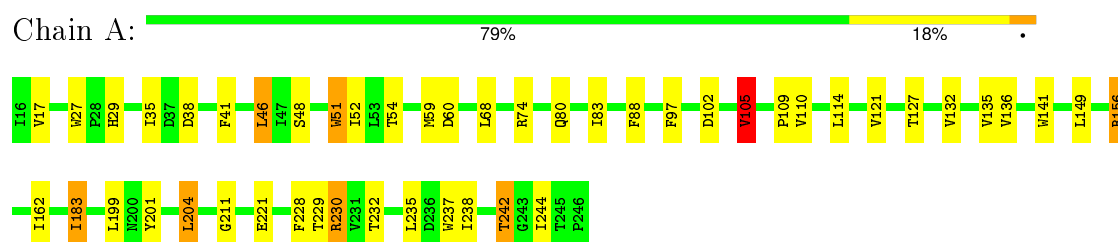
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	52	Total	O	0	0
			52	52		
3	B	47	Total	O	0	0
			47	47		
3	C	22	Total	O	0	0
			22	22		
3	D	19	Total	O	0	0
			19	19		

3 Residue-property plots [i](#)

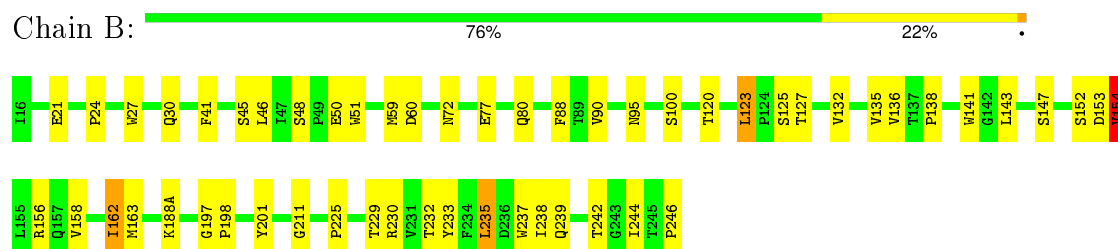
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

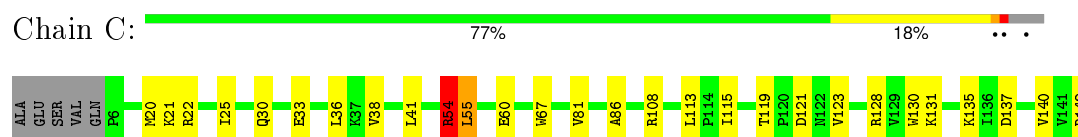
• Molecule 1: COLLAGENASE



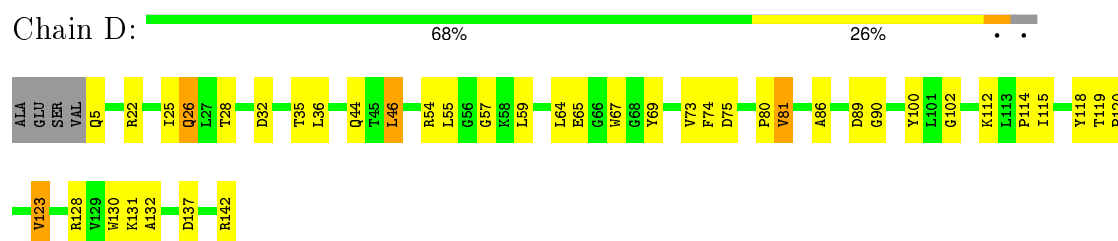
• Molecule 1: COLLAGENASE



• Molecule 2: ECOTIN



• Molecule 2: ECOTIN



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	89.11Å 89.11Å 291.55Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.30)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.189 , 0.238	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5527	wwPDB-VP
Average B, all atoms (Å ²)	20.0	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	0.73	0/1691	1.43	19/2322 (0.8%)
1	B	0.73	0/1691	1.41	21/2322 (0.9%)
2	C	0.68	0/1070	1.40	9/1455 (0.6%)
2	D	0.70	0/1055	1.48	15/1441 (1.0%)
All	All	0.71	0/5507	1.43	64/7540 (0.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	1

There are no bond length outliers.

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	128	ARG	NE-CZ-NH2	-10.70	114.95	120.30
1	B	156	ARG	NE-CZ-NH2	-9.48	115.56	120.30
1	A	230	ARG	NE-CZ-NH2	-9.30	115.65	120.30
2	D	67	TRP	CD1-CG-CD2	9.05	113.54	106.30
2	C	22	ARG	NE-CZ-NH2	-8.77	115.92	120.30
1	B	51	TRP	CD1-CG-CD2	8.57	113.16	106.30
1	A	141	TRP	CD1-CG-CD2	8.52	113.11	106.30
1	B	51	TRP	CE2-CD2-CG	-8.38	100.59	107.30
1	A	74	ARG	NE-CZ-NH2	-8.21	116.19	120.30
1	B	237	TRP	CD1-CG-CD2	8.21	112.87	106.30
1	A	74	ARG	NE-CZ-NH1	8.18	124.39	120.30
2	C	67	TRP	CD1-CG-CD2	8.16	112.83	106.30
1	A	51	TRP	CD1-CG-CD2	8.00	112.70	106.30
1	B	27	TRP	CD1-CG-CD2	7.92	112.64	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	141	TRP	CD1-CG-CD2	7.79	112.53	106.30
1	A	51	TRP	CE2-CD2-CG	-7.76	101.09	107.30
1	A	27	TRP	CD1-CG-CD2	7.74	112.50	106.30
2	C	130	TRP	CD1-CG-CD2	7.56	112.35	106.30
2	D	67	TRP	CE2-CD2-CG	-7.48	101.32	107.30
1	B	141	TRP	CE2-CD2-CG	-7.44	101.35	107.30
1	A	27	TRP	CE2-CD2-CG	-7.38	101.39	107.30
1	A	141	TRP	CE2-CD2-CG	-7.31	101.45	107.30
2	C	130	TRP	CE2-CD2-CG	-7.27	101.49	107.30
1	B	237	TRP	CE2-CD2-CG	-7.26	101.49	107.30
1	A	156	ARG	NE-CZ-NH2	-7.25	116.68	120.30
1	B	27	TRP	CE2-CD2-CG	-7.11	101.61	107.30
1	A	237	TRP	CD1-CG-CD2	7.11	111.99	106.30
2	C	67	TRP	CE2-CD2-CG	-6.98	101.72	107.30
2	C	54	ARG	NE-CZ-NH2	-6.96	116.82	120.30
2	D	130	TRP	CD1-CG-CD2	6.93	111.85	106.30
1	A	237	TRP	CE2-CD2-CG	-6.92	101.76	107.30
2	D	130	TRP	CE2-CD2-CG	-6.92	101.77	107.30
2	D	112	LYS	CA-CB-CG	6.91	128.61	113.40
1	B	156	ARG	CG-CD-NE	-6.84	97.44	111.80
2	D	90	GLY	CA-C-N	-6.68	102.50	117.20
1	B	59	MET	CG-SD-CE	-6.16	90.34	100.20
1	A	242	THR	N-CA-CB	-5.95	98.99	110.30
1	B	51	TRP	CG-CD2-CE3	5.95	139.25	133.90
1	B	51	TRP	CB-CG-CD1	-5.90	119.33	127.00
2	D	123	VAL	CG1-CB-CG2	-5.86	101.52	110.90
1	B	154	VAL	N-CA-CB	-5.72	98.92	111.50
1	A	102	ASP	CB-CG-OD1	5.69	123.42	118.30
1	A	51	TRP	CG-CD2-CE3	5.67	139.00	133.90
1	B	141	TRP	CB-CG-CD1	-5.64	119.67	127.00
2	D	69	TYR	CB-CG-CD2	-5.62	117.63	121.00
2	D	128	ARG	NH1-CZ-NH2	5.52	125.47	119.40
2	D	67	TRP	CG-CD1-NE1	-5.46	104.64	110.10
2	D	54	ARG	NE-CZ-NH2	-5.43	117.59	120.30
1	A	105	VAL	N-CA-CB	-5.42	99.58	111.50
1	B	141	TRP	CG-CD2-CE3	5.42	138.78	133.90
2	D	46	LEU	CA-CB-CG	5.35	127.60	115.30
2	C	60	GLU	CA-CB-CG	5.31	125.07	113.40
1	A	27	TRP	CG-CD2-CE3	5.29	138.66	133.90
1	A	51	TRP	CB-CG-CD1	-5.29	120.13	127.00
1	B	230	ARG	CA-CB-CG	5.28	125.02	113.40
1	B	237	TRP	CG-CD1-NE1	-5.25	104.85	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	204	LEU	CA-CB-CG	5.25	127.37	115.30
2	C	38	VAL	CG1-CB-CG2	-5.19	102.60	110.90
1	B	233	TYR	CB-CG-CD1	-5.18	117.89	121.00
1	B	143	LEU	CA-CB-CG	5.16	127.17	115.30
2	D	112	LYS	CB-CA-C	-5.12	100.17	110.40
2	C	130	TRP	CG-CD2-CE3	5.10	138.49	133.90
2	D	81	VAL	N-CA-CB	-5.06	100.37	111.50
1	B	46	LEU	CA-CB-CG	5.04	126.88	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	5	GLN	Peptide

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	1653	0	1571	22	0
1	B	1653	0	1571	18	0
2	C	1048	0	1021	15	0
2	D	1033	0	981	14	0
3	A	52	0	0	2	0
3	B	47	0	0	1	0
3	C	22	0	0	0	0
3	D	19	0	0	0	0
All	All	5527	0	5144	64	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 6.

All (64) 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)
2:D:119:THR:HB	2:D:123:VAL:HG23	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:ILE:HD11	1:A:109:PRO:HD2	1.65	0.77
1:A:48:SER:HB3	1:A:244:ILE:HD11	1.66	0.76
2:D:44:GLN:HG3	2:D:123:VAL:HG12	1.73	0.71
1:B:242:THR:HG22	1:B:244:ILE:HG12	1.76	0.67
1:A:97:PHE:O	2:C:54:ARG:HD2	1.94	0.67
2:C:128:ARG:HD3	2:D:132:ALA:HB1	1.77	0.65
1:A:54:THR:HG21	1:A:59:MET:HE3	1.79	0.65
1:B:136:VAL:HG12	1:B:201:TYR:HB2	1.82	0.61
1:A:136:VAL:HG12	1:A:201:TYR:HB2	1.80	0.61
1:A:48:SER:CB	1:A:244:ILE:HD11	2.35	0.56
1:A:132:VAL:HA	1:A:162:ILE:HG22	1.89	0.54
2:D:26:GLN:NE2	2:D:114:PRO:HB3	2.23	0.53
1:A:17:VAL:HG11	1:A:221:GLU:HG2	1.90	0.53
2:D:35:THR:OG1	2:D:131:LYS:NZ	2.42	0.52
1:B:21:GLU:HG3	1:B:154:VAL:HG13	1.92	0.52
1:B:123:LEU:HD22	1:B:244:ILE:HG22	1.91	0.52
1:A:17:VAL:CG1	1:A:221:GLU:HG2	2.40	0.52
1:B:30:GLN:NE2	1:B:198:PRO:HD2	2.25	0.51
2:C:135:LYS:NZ	2:C:137:ASP:HB2	2.25	0.51
2:C:135:LYS:HZ2	2:C:137:ASP:HB2	1.76	0.50
2:C:119:THR:HB	2:C:123:VAL:CG2	2.42	0.50
1:B:238:ILE:O	1:B:242:THR:HB	2.11	0.50
2:C:119:THR:HB	2:C:123:VAL:HG22	1.93	0.49
2:C:30:GLN:HG3	2:C:36:LEU:HD21	1.94	0.49
1:A:29:HIS:CG	1:A:121:VAL:HB	2.47	0.49
1:B:72:ASN:HA	1:B:153:ASP:O	2.12	0.49
2:D:36:LEU:HD23	2:D:131:LYS:HG3	1.94	0.48
2:D:57:GLY:HA3	2:D:74:PHE:CE1	2.49	0.48
1:A:211:GLY:HA2	1:A:229:THR:O	2.14	0.47
2:D:119:THR:HB	2:D:123:VAL:CG2	2.39	0.47
2:C:21:LYS:HB2	2:C:121:ASP:HA	1.97	0.47
2:C:30:GLN:HB2	2:C:33:GLU:HG2	1.98	0.46
1:B:163:MET:SD	1:B:225:PRO:HB3	2.55	0.46
2:C:140:VAL:HG12	2:C:142:ARG:HG3	1.97	0.45
1:A:238:ILE:O	1:A:242:THR:HB	2.16	0.45
1:A:46:LEU:HD22	1:A:48:SER:O	2.16	0.45
1:B:158:VAL:HG21	1:B:188(A):LYS:HB3	1.97	0.45
1:B:211:GLY:HA2	1:B:229:THR:O	2.17	0.45
1:A:48:SER:HB3	1:A:244:ILE:CD1	2.44	0.44
1:A:156:ARG:HD3	3:A:247:HOH:O	2.16	0.44
2:D:100:TYR:CZ	2:D:102:GLY:HA2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:THR:HA	1:B:235:LEU:HD22	2.00	0.43
1:A:183:ILE:HB	1:A:228:PHE:HE1	1.84	0.43
1:B:41:PHE:HB3	2:D:86:ALA:HB3	2.00	0.43
1:A:68:LEU:O	1:A:80:GLN:HA	2.19	0.43
1:A:232:THR:HA	1:A:235:LEU:HG	2.01	0.42
1:B:95:ASN:HB3	1:B:100:SER:OG	2.20	0.42
1:A:46:LEU:HD23	1:A:52:ILE:HD13	2.01	0.42
1:B:197:GLY:HA3	3:B:259:HOH:O	2.19	0.42
2:D:25:ILE:HB	2:D:115:ILE:HB	2.02	0.42
1:A:51:TRP:CE3	1:A:105:VAL:HG13	2.54	0.42
1:A:41:PHE:HB3	2:C:86:ALA:HB3	2.00	0.42
1:B:45:SER:OG	1:B:198:PRO:HB3	2.20	0.41
1:B:138:PRO:HD2	1:B:158:VAL:O	2.20	0.41
1:A:230:ARG:NH2	3:A:297:HOH:O	2.52	0.41
2:C:142:ARG:OXT	2:D:22:ARG:NH1	2.54	0.41
2:D:55:LEU:HD13	2:D:80:PRO:HG3	2.01	0.41
2:D:22:ARG:HD3	2:D:118:TYR:CZ	2.56	0.41
2:C:25:ILE:HB	2:C:115:ILE:HB	2.03	0.41
1:B:132:VAL:HA	1:B:162:ILE:HG13	2.03	0.41
2:C:20:MET:HA	2:C:119:THR:O	2.21	0.41
1:B:77:GLU:HB2	1:B:80:GLN:HG3	2.02	0.41
2:C:54:ARG:HG3	2:C:55:LEU:N	2.36	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	224/226 (99%)	216 (96%)	6 (3%)	2 (1%)	21	24
1	B	224/226 (99%)	213 (95%)	10 (4%)	1 (0%)	39	48
2	C	135/142 (95%)	131 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	136/142 (96%)	130 (96%)	5 (4%)	1 (1%)	26	31
All	All	719/736 (98%)	690 (96%)	25 (4%)	4 (1%)	30	36

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	ASP
1	B	60	ASP
2	D	89	ASP
1	A	38	ASP

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	179/179 (100%)	167 (93%)	12 (7%)	20	26
1	B	179/179 (100%)	162 (90%)	17 (10%)	11	12
2	C	109/125 (87%)	102 (94%)	7 (6%)	22	28
2	D	104/125 (83%)	91 (88%)	13 (12%)	6	6
All	All	571/608 (94%)	522 (91%)	49 (9%)	13	15

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ILE
1	A	46	LEU
1	A	88	PHE
1	A	105	VAL
1	A	110	VAL
1	A	114	LEU
1	A	127	THR
1	A	135	VAL
1	A	149	LEU
1	A	183	ILE

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Mol	Chain	Res	Type
1	A	199	LEU
1	A	204	LEU
1	B	24	PRO
1	B	48	SER
1	B	50	GLU
1	B	88	PHE
1	B	90	VAL
1	B	120	THR
1	B	123	LEU
1	B	125	SER
1	B	127	THR
1	B	135	VAL
1	B	147	SER
1	B	152	SER
1	B	154	VAL
1	B	162	ILE
1	B	235	LEU
1	B	239	GLN
1	B	246	PRO
2	C	41	LEU
2	C	54	ARG
2	C	55	LEU
2	C	81	VAL
2	C	108	ARG
2	C	113	LEU
2	C	131	LYS
2	D	26	GLN
2	D	28	THR
2	D	32	ASP
2	D	46	LEU
2	D	59	LEU
2	D	64	LEU
2	D	65	GLU
2	D	73	VAL
2	D	75	ASP
2	D	81	VAL
2	D	120	PRO
2	D	137	ASP
2	D	142	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	HIS
1	A	101	ASN
1	B	30	GLN
2	C	23	GLN
2	C	26	GLN
2	C	61	ASN
2	D	23	GLN
2	D	26	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 ⓘ

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.