



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:33 PM GMT

PDB ID : 4CMS
Title : X-RAY ANALYSES OF ASPARTIC PROTEINASES IV. STRUCTURE AND REFINEMENT AT 2.2 ANGSTROMS RESOLUTION OF BOVINE CHYMOSIN
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Deposited on : 1991-11-01
Resolution : 2.20 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

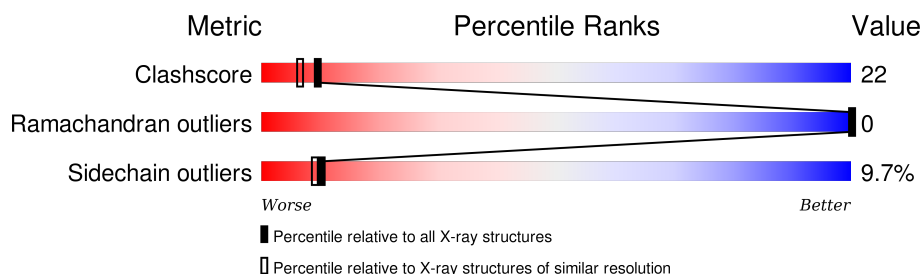
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)

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	323	 50% 37% 11% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2618 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 CHYMOSIN B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	320	Total	C	N	O	S	0	0	0
			2487	1585	395	493	14			

- Molecule 2 is water.

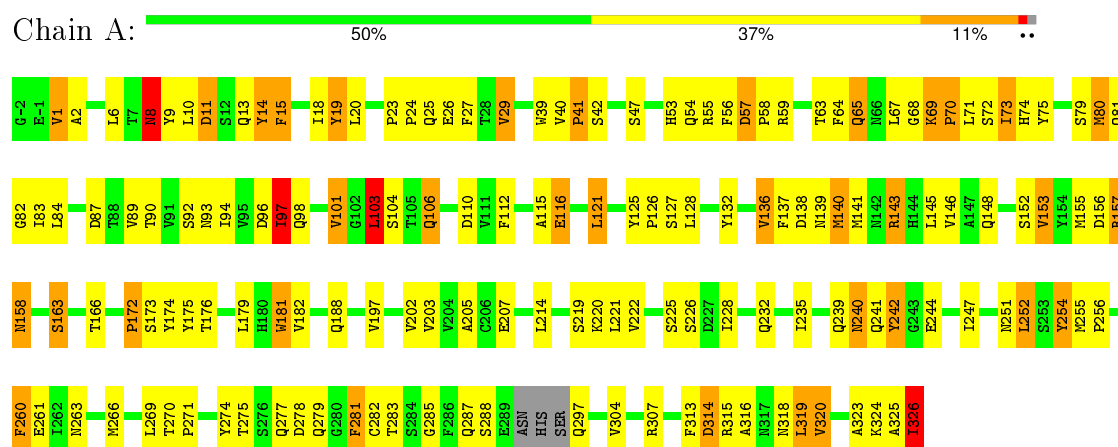
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	131	Total	O	0	0
			131	131		

3 Residue-property plots

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: CHYMOSIN B



4 Data and refinement statistics

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

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	79.98 Å 114.12 Å 72.76 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	RESTRAIN	Depositor
R, R_{free}	0.158 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2618	wwPDB-VP
Average B, all atoms (Å ²)	0.0	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	1.17	5/2548 (0.2%)	1.91	59/3469 (1.7%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	181	TRP	NE1-CE2	-5.31	1.30	1.37
1	A	39	TRP	NE1-CE2	-5.29	1.30	1.37
1	A	326	ILE	C-OXT	5.28	1.33	1.23
1	A	297	GLN	CD-OE1	5.17	1.35	1.24
1	A	106	GLN	CD-OE1	5.02	1.34	1.24

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	141	MET	CG-SD-CE	12.36	119.97	100.20
1	A	87	ASP	CB-CG-OD2	11.70	128.83	118.30
1	A	1	VAL	CA-CB-CG1	9.45	125.08	110.90
1	A	29	VAL	CA-CB-CG1	8.83	124.15	110.90
1	A	103	LEU	CB-CG-CD2	8.16	124.87	111.00
1	A	59	ARG	NE-CZ-NH2	-8.06	116.27	120.30
1	A	59	ARG	NE-CZ-NH1	7.94	124.27	120.30
1	A	202	VAL	CA-CB-CG2	7.84	122.65	110.90
1	A	222	VAL	CA-CB-CG2	7.75	122.52	110.90
1	A	158	ASN	C-N-CA	7.71	138.50	122.30
1	A	101	VAL	CA-CB-CG2	7.61	122.32	110.90
1	A	59	ARG	CD-NE-CZ	-7.51	113.09	123.60
1	A	40	VAL	CA-CB-CG2	7.47	122.11	110.90
1	A	136	VAL	CA-CB-CG2	7.39	121.99	110.90
1	A	19	TYR	CA-CB-CG	-7.32	99.48	113.40
1	A	255	MET	CG-SD-CE	7.18	111.69	100.20
1	A	143	ARG	CD-NE-CZ	-6.97	113.84	123.60
1	A	138	ASP	CB-CG-OD1	-6.87	112.12	118.30
1	A	153	VAL	CA-CB-CG2	6.86	121.18	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	14	TYR	CB-CG-CD2	-6.84	116.89	121.00
1	A	57	ASP	CB-CG-OD2	6.82	124.44	118.30
1	A	254	TYR	CB-CG-CD2	-6.35	117.19	121.00
1	A	157	ARG	NE-CZ-NH1	-6.30	117.15	120.30
1	A	41	PRO	C-N-CA	6.13	137.02	121.70
1	A	15	PHE	CG-CD2-CE2	-6.11	114.07	120.80
1	A	266	MET	CG-SD-CE	6.08	109.93	100.20
1	A	155	MET	CG-SD-CE	6.03	109.84	100.20
1	A	314	ASP	CB-CA-C	5.99	122.39	110.40
1	A	70	PRO	CA-N-CD	5.98	120.08	111.70
1	A	260	PHE	CB-CG-CD2	-5.97	116.62	120.80
1	A	55	ARG	CA-CB-CG	-5.95	100.32	113.40
1	A	140	MET	CG-SD-CE	5.87	109.60	100.20
1	A	176	THR	CA-CB-CG2	5.85	120.59	112.40
1	A	240	ASN	C-N-CA	5.80	136.21	121.70
1	A	315	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	A	320	VAL	CA-CB-CG2	5.75	119.52	110.90
1	A	65	GLN	N-CA-CB	5.71	120.88	110.60
1	A	97	ILE	O-C-N	-5.67	113.63	122.70
1	A	261	GLU	OE1-CD-OE2	-5.60	116.58	123.30
1	A	176	THR	CA-CB-OG1	5.57	120.69	109.00
1	A	304	VAL	CA-CB-CG2	5.57	119.25	110.90
1	A	29	VAL	CA-CB-CG2	5.51	119.16	110.90
1	A	80	MET	O-C-N	5.46	131.44	122.70
1	A	148	GLN	N-CA-CB	5.42	120.35	110.60
1	A	80	MET	N-CA-C	-5.40	96.42	111.00
1	A	263	ASN	CB-CA-C	5.34	121.07	110.40
1	A	80	MET	CG-SD-CE	5.32	108.71	100.20
1	A	319	LEU	CB-CG-CD2	5.30	120.00	111.00
1	A	110	ASP	O-C-N	5.27	131.13	122.70
1	A	47	SER	O-C-N	-5.27	114.27	122.70
1	A	137	PHE	CZ-CE2-CD2	5.26	126.42	120.10
1	A	172	PRO	C-N-CA	5.26	134.84	121.70
1	A	15	PHE	CB-CG-CD2	-5.17	117.18	120.80
1	A	137	PHE	CG-CD2-CE2	-5.16	115.12	120.80
1	A	121	LEU	C-N-CA	5.15	133.11	122.30
1	A	96	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	8	ASN	N-CA-CB	5.11	119.79	110.60
1	A	87	ASP	OD1-CG-OD2	-5.07	113.66	123.30
1	A	75	TYR	O-C-N	-5.06	114.60	123.20

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	2487	0	2364	109	0
2	A	131	0	0	6	0
All	All	2618	0	2364	109	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 22.

All (109) 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:10:LEU:O	1:A:11:ASP:CB	2.06	1.03
1:A:10:LEU:O	1:A:11:ASP:HB2	1.22	1.02
1:A:278:ASP:HB2	1:A:281:PHE:CE2	1.98	0.97
1:A:69:LYS:HG2	1:A:132:TYR:CD2	1.99	0.97
1:A:73:ILE:HD13	2:A:1008:HOH:O	1.64	0.95
1:A:140:MET:HA	1:A:145:LEU:HD12	1.56	0.88
1:A:278:ASP:O	1:A:279:GLN:HG2	1.75	0.86
1:A:41:PRO:HA	1:A:104:SER:OG	1.79	0.82
1:A:251:ASN:ND2	1:A:254:TYR:HD1	1.79	0.79
1:A:2:ALA:HB1	1:A:92:SER:HB3	1.64	0.78
1:A:69:LYS:CG	1:A:132:TYR:CD2	2.66	0.78
1:A:247:ILE:O	1:A:282:CYS:HB2	1.84	0.77
1:A:20:LEU:HD13	1:A:89:VAL:HG22	1.65	0.77
1:A:270:THR:HB	1:A:271:PRO:HD2	1.66	0.76
1:A:25:GLN:HE22	1:A:57:ASP:H	1.31	0.75
1:A:278:ASP:HB2	1:A:281:PHE:CD2	2.23	0.74
1:A:277:GLN:HB2	1:A:282:CYS:SG	2.28	0.74
1:A:15:PHE:CE2	1:A:116:GLU:HB3	2.24	0.73
1:A:278:ASP:HB2	1:A:281:PHE:HE2	1.53	0.69
1:A:20:LEU:HD21	1:A:101:VAL:HG21	1.75	0.68
1:A:220:LYS:HG3	1:A:287:GLN:OE1	1.92	0.68
1:A:251:ASN:ND2	1:A:254:TYR:CD1	2.61	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:ASN:O	1:A:143:ARG:HD2	1.94	0.67
1:A:324:LYS:HE2	2:A:1105:HOH:O	1.94	0.67
1:A:270:THR:CB	1:A:271:PRO:HD2	2.29	0.62
1:A:228:ILE:O	1:A:232:GLN:HG2	2.00	0.61
1:A:203:VAL:HG12	1:A:207:GLU:HG2	1.82	0.61
1:A:278:ASP:O	1:A:281:PHE:HD2	1.84	0.59
1:A:2:ALA:HB1	1:A:92:SER:CB	2.30	0.59
1:A:316:ALA:HB3	2:A:1015:HOH:O	2.03	0.58
1:A:326:ILE:CG2	2:A:1064:HOH:O	2.52	0.58
1:A:69:LYS:HB3	1:A:84:LEU:HD12	1.85	0.57
1:A:203:VAL:CG1	1:A:207:GLU:HG2	2.34	0.57
1:A:15:PHE:CZ	1:A:116:GLU:HB3	2.39	0.57
1:A:9:TYR:HB2	1:A:15:PHE:CZ	2.40	0.56
1:A:6:LEU:HB2	1:A:163:SER:HB2	1.87	0.56
1:A:271:PRO:HA	1:A:274:TYR:CZ	2.41	0.56
1:A:69:LYS:HD2	1:A:69:LYS:N	2.19	0.55
1:A:11:ASP:O	1:A:307:ARG:NH2	2.40	0.55
1:A:127:SER:OG	1:A:188:GLN:HG2	2.07	0.55
1:A:156:ASP:OD2	1:A:158:ASN:HB2	2.07	0.54
1:A:42:SER:HB2	1:A:103:LEU:HD13	1.90	0.54
1:A:270:THR:HB	1:A:271:PRO:CD	2.37	0.54
1:A:239:GLN:HA	1:A:244:GLU:O	2.08	0.53
1:A:270:THR:CB	1:A:271:PRO:CD	2.87	0.53
1:A:19:TYR:HB2	1:A:90:THR:HB	1.91	0.52
1:A:19:TYR:HA	1:A:25:GLN:O	2.10	0.51
1:A:313:PHE:N	1:A:313:PHE:CD1	2.78	0.51
1:A:81:GLN:NE2	2:A:1033:HOH:O	2.44	0.50
1:A:19:TYR:CE1	1:A:26:GLU:HG3	2.46	0.50
1:A:220:LYS:HB3	1:A:285:GLY:O	2.12	0.50
1:A:20:LEU:CD1	1:A:89:VAL:HG22	2.38	0.50
1:A:172:PRO:HA	1:A:175:TYR:CE2	2.47	0.50
1:A:97:ILE:O	1:A:98:GLN:C	2.50	0.49
1:A:8:ASN:HB3	1:A:14:TYR:CD2	2.48	0.49
1:A:181:TRP:HB3	1:A:319:LEU:HD13	1.95	0.49
1:A:260:PHE:HE2	1:A:269:LEU:HD12	1.77	0.49
1:A:225:SER:HA	1:A:288:SER:OG	2.14	0.48
1:A:153:VAL:HG23	1:A:313:PHE:HE1	1.79	0.47
1:A:2:ALA:CB	1:A:92:SER:HB3	2.41	0.47
1:A:80:MET:HE2	1:A:104:SER:HA	1.96	0.47
1:A:68:GLY:O	1:A:83:ILE:HG23	2.15	0.47
1:A:69:LYS:HA	1:A:70:PRO:HD3	1.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:VAL:HG12	1:A:207:GLU:CG	2.44	0.47
1:A:271:PRO:O	1:A:275:THR:CB	2.65	0.45
1:A:314:ASP:O	1:A:318:ASN:CA	2.64	0.45
1:A:240:ASN:N	1:A:244:GLU:O	2.44	0.45
1:A:9:TYR:HB2	1:A:15:PHE:CE2	2.52	0.45
1:A:157:ARG:HD2	1:A:157:ARG:HH11	1.56	0.45
1:A:69:LYS:HG3	1:A:132:TYR:CD2	2.50	0.45
1:A:81:GLN:HB3	1:A:106:GLN:HB2	1.98	0.45
1:A:324:LYS:HG3	1:A:325:ALA:N	2.30	0.44
1:A:41:PRO:HA	1:A:104:SER:HG	1.79	0.44
1:A:271:PRO:HA	1:A:274:TYR:CE1	2.53	0.44
1:A:74:HIS:CE1	1:A:79:SER:OG	2.71	0.43
1:A:232:GLN:OE1	1:A:232:GLN:HA	2.18	0.43
1:A:83:ILE:HD12	1:A:83:ILE:HG23	1.69	0.43
1:A:314:ASP:O	1:A:318:ASN:HA	2.18	0.43
1:A:69:LYS:CG	1:A:132:TYR:CE2	3.01	0.43
1:A:252:LEU:HD11	1:A:275:THR:HG21	2.01	0.43
1:A:64:PHE:CG	1:A:65:GLN:N	2.86	0.43
1:A:53:HIS:HE1	1:A:112:PHE:O	2.02	0.43
1:A:197:VAL:HB	1:A:205:ALA:HB3	2.01	0.43
1:A:69:LYS:HG2	1:A:132:TYR:CG	2.51	0.43
1:A:82:GLY:O	1:A:83:ILE:HD13	2.18	0.42
1:A:56:PHE:O	1:A:58:PRO:HD3	2.19	0.42
1:A:214:LEU:HA	1:A:214:LEU:HD12	1.76	0.42
1:A:157:ARG:HG3	1:A:158:ASN:N	2.35	0.42
1:A:271:PRO:O	1:A:275:THR:HB	2.19	0.42
1:A:260:PHE:N	1:A:260:PHE:CD2	2.87	0.42
1:A:153:VAL:HG23	1:A:313:PHE:CE1	2.53	0.42
1:A:121:LEU:HD11	1:A:136:VAL:HG21	2.02	0.42
1:A:81:GLN:CB	1:A:106:GLN:HB2	2.50	0.42
1:A:27:PHE:CE1	1:A:54:GLN:HB3	2.55	0.42
1:A:219:SER:HB2	2:A:1104:HOH:O	2.19	0.42
1:A:182:VAL:N	1:A:320:VAL:O	2.45	0.42
1:A:116:GLU:OE1	1:A:116:GLU:HA	2.20	0.41
1:A:9:TYR:HB3	1:A:13:GLN:HB2	2.01	0.41
1:A:19:TYR:CD2	1:A:19:TYR:N	2.88	0.41
1:A:174:TYR:HD2	1:A:174:TYR:HA	1.58	0.41
1:A:2:ALA:HB2	1:A:94:ILE:HG13	2.02	0.41
1:A:152:SER:HB2	1:A:166:THR:HB	2.03	0.41
1:A:9:TYR:HB2	1:A:15:PHE:HZ	1.81	0.41
1:A:13:GLN:HE22	1:A:115:ALA:HA	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:ASN:ND2	1:A:242:TYR:HB2	2.36	0.40
1:A:179:LEU:HA	1:A:323:ALA:HB2	2.02	0.40
1:A:235:ILE:HG22	1:A:256:PRO:HG2	2.03	0.40
1:A:125:TYR:HB3	1:A:126:PRO:HD2	2.04	0.40
1:A:23:PRO:HB2	1:A:24:PRO:HD2	2.03	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	316/323 (98%)	306 (97%)	10 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	277/280 (99%)	250 (90%)	27 (10%)	10	9

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	VAL

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Mol	Chain	Res	Type
1	A	8	ASN
1	A	11	ASP
1	A	18	ILE
1	A	29	VAL
1	A	63	THR
1	A	67	LEU
1	A	69	LYS
1	A	71	LEU
1	A	72	SER
1	A	73	ILE
1	A	93	ASN
1	A	97	ILE
1	A	103	LEU
1	A	116	GLU
1	A	128	LEU
1	A	146	VAL
1	A	163	SER
1	A	173	SER
1	A	221	LEU
1	A	226	SER
1	A	241	GLN
1	A	242	TYR
1	A	252	LEU
1	A	281	PHE
1	A	283	THR
1	A	326	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	48	ASN
1	A	54	GLN
1	A	99	GLN
1	A	139	ASN
1	A	142	ASN
1	A	251	ASN

5.3.3 RNA ⓘ

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 carbohydrates 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 will therefore be empty.

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

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

6.3 Carbohydrates [i](#)

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

6.4 Ligands [i](#)

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

6.5 Other polymers [i](#)

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