



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:30 AM UTC

PDB ID : 2BEB / pdb\_00002beb  
Title : X-ray structure of Asn to Thr mutant of Winged Bean Chymotrypsin inhibitor  
Authors : Dattagupta, J.K.; Sen, U.; Dasgupta, J.; Khamrui, S.  
Deposited on : 2005-10-24  
Resolution : 2.81 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](mailto: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>.

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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

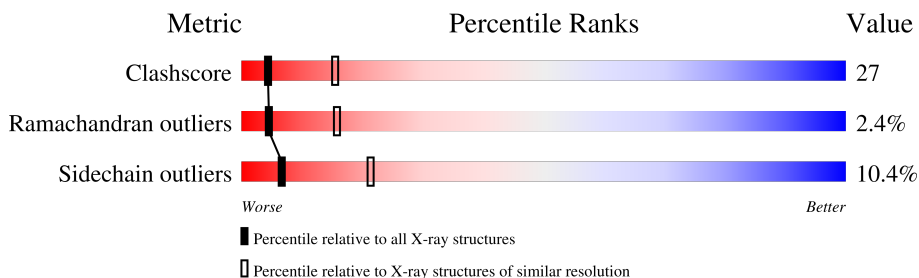
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.81 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	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)

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  $\geq 3$ , 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	186	 45%                      41%                      5% • 9%
1	B	186	 48%                      37%                      6% • 7%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2938 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 Chymotrypsin inhibitor 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	170	1317	840	229	244	4	0	0	0
1	B	173	1352	862	233	253	4	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	cloning artifact	UNP P10822
A	2	GLU	-	cloning artifact	UNP P10822
A	3	PHE	-	cloning artifact	UNP P10822
A	17	THR	ASN	engineered mutation	UNP P10822
B	1	MET	-	cloning artifact	UNP P10822
B	2	GLU	-	cloning artifact	UNP P10822
B	3	PHE	-	cloning artifact	UNP P10822
B	17	THR	ASN	engineered mutation	UNP P10822

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	126	Total	O	0	0
			126	126		
2	B	143	Total	O	0	0
			143	143		

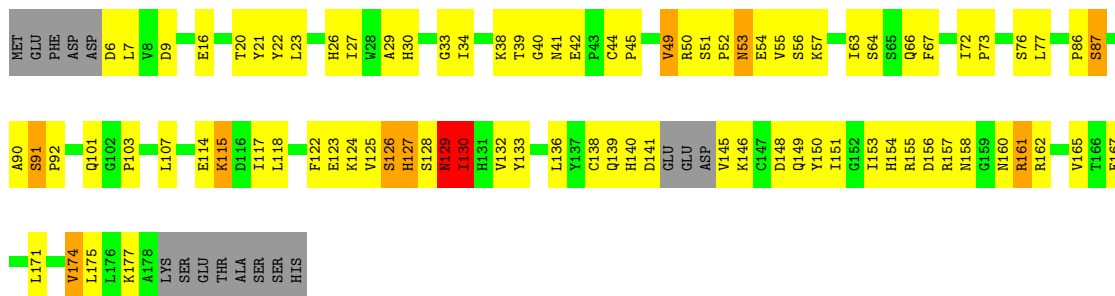
### 3 Residue-property plots [i](#)

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.

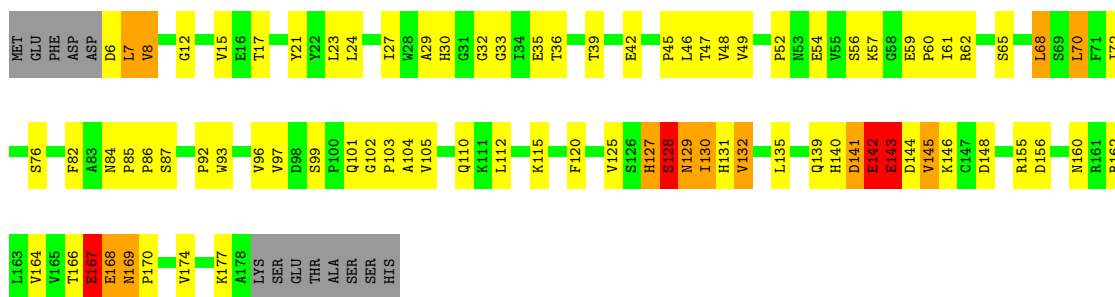
- Molecule 1: Chymotrypsin inhibitor 3

Chain A: 



- Molecule 1: Chymotrypsin inhibitor 3

Chain B: 



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.50Å 129.55Å 36.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.91 – 2.81	Depositor
% Data completeness (in resolution range)	94.4 (14.91-2.81)	Depositor
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.201 , 0.254	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	2938	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	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	0.44	0/1348	1.12	11/1834 (0.6%)
1	B	0.55	1/1386 (0.1%)	1.52	20/1888 (1.1%)
All	All	0.50	1/2734 (0.0%)	1.34	31/3722 (0.8%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	143	GLU	CA-CB	5.73	1.63	1.53

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	140	HIS	CA-C-N	-18.45	98.06	122.79
1	B	140	HIS	C-N-CA	-18.45	98.06	122.79
1	B	141	ASP	N-CA-C	13.92	128.88	109.11
1	B	166	THR	N-CA-C	13.90	132.04	109.95
1	B	129	ASN	N-CA-C	-13.69	96.62	113.18
1	B	169	ASN	CA-C-N	10.41	132.85	119.84
1	B	169	ASN	C-N-CA	10.41	132.85	119.84
1	B	140	HIS	CB-CA-C	-10.26	98.17	111.40
1	B	140	HIS	N-CA-C	9.10	124.02	111.55
1	B	169	ASN	N-CA-C	8.49	128.58	109.81
1	A	128	SER	N-CA-C	8.43	122.59	109.52
1	B	145	VAL	N-CA-C	8.10	122.31	108.95
1	B	139	GLN	N-CA-C	7.63	121.68	109.86
1	B	166	THR	CA-C-N	7.39	134.09	122.26
1	B	166	THR	C-N-CA	7.39	134.09	122.26
1	A	107	LEU	N-CA-C	-7.12	99.10	110.14
1	A	130	ILE	N-CA-C	-6.73	95.34	109.34
1	B	84	ASN	CA-C-N	6.54	127.12	120.38
1	B	84	ASN	C-N-CA	6.54	127.12	120.38
1	A	91	SER	CA-C-N	6.31	127.46	120.45
1	A	91	SER	C-N-CA	6.31	127.46	120.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	49	VAL	N-CA-C	6.05	117.55	108.96
1	B	127	HIS	N-CA-C	5.96	119.44	107.41
1	A	29	ALA	N-CA-C	-5.79	106.84	114.31
1	A	117	ILE	N-CA-C	-5.75	107.90	113.53
1	B	167	GLU	N-CA-CB	-5.60	102.51	110.58
1	A	129	ASN	CA-C-N	5.56	131.98	121.97
1	A	129	ASN	C-N-CA	5.56	131.98	121.97
1	A	174	VAL	N-CA-C	-5.47	100.36	108.45
1	B	142	GLU	N-CA-C	5.29	122.06	110.80
1	B	93	TRP	N-CA-C	5.08	118.00	110.48

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	1317	0	1315	72	0
1	B	1352	0	1340	70	0
2	A	126	0	0	17	0
2	B	143	0	0	16	0
All	All	2938	0	2655	142	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 27.

All (142) 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:127:HIS:NE2	1:A:130:ILE:HB	1.63	1.13
1:B:146:LYS:HE2	1:B:148:ASP:HB3	1.36	1.05
1:B:76:SER:HB3	2:B:682:HOH:O	1.63	0.97
1:B:27:ILE:HG13	2:B:685:HOH:O	1.68	0.92
1:A:139:GLN:O	1:A:145:VAL:HA	1.74	0.87
1:A:73:PRO:HG3	2:A:717:HOH:O	1.77	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:LYS:CE	1:B:148:ASP:HB3	2.09	0.82
1:A:53:ASN:HD22	1:A:53:ASN:N	1.79	0.77
1:B:125:VAL:HG12	1:B:127:HIS:H	1.50	0.77
1:A:127:HIS:CD2	1:A:127:HIS:C	2.63	0.76
1:B:162:ARG:HD3	2:B:726:HOH:O	1.86	0.74
1:B:52:PRO:HD2	2:B:462:HOH:O	1.88	0.72
1:A:139:GLN:HG3	2:A:418:HOH:O	1.89	0.71
1:B:39:THR:O	1:B:42:GLU:HB2	1.90	0.71
1:B:42:GLU:HG2	1:B:46:LEU:HD12	1.71	0.71
1:A:90:ALA:HB3	2:A:609:HOH:O	1.90	0.71
1:B:30:HIS:HB3	1:B:54:GLU:OE2	1.92	0.69
1:A:27:ILE:HB	1:A:30:HIS:HD2	1.58	0.69
1:B:167:GLU:O	1:B:168:GLU:HB2	1.91	0.68
1:A:157:ARG:NH1	1:A:158:ASN:HD21	1.92	0.68
1:B:155:ARG:HD2	2:B:399:HOH:O	1.93	0.68
1:A:103:PRO:HB2	1:A:165:VAL:CG2	2.24	0.68
1:B:129:ASN:HA	2:B:608:HOH:O	1.95	0.67
1:A:129:ASN:O	1:A:130:ILE:HG12	1.93	0.67
1:B:60:PRO:HD2	2:B:446:HOH:O	1.94	0.66
1:B:29:ALA:O	2:B:685:HOH:O	2.13	0.65
1:A:86:PRO:HG3	2:A:421:HOH:O	1.96	0.65
1:B:47:THR:HG22	1:B:49:VAL:HG13	1.80	0.64
1:B:146:LYS:HG2	2:B:479:HOH:O	1.97	0.63
1:A:44:CYS:HB2	2:A:713:HOH:O	1.97	0.63
1:A:38:LYS:HG3	1:A:44:CYS:O	1.99	0.62
1:A:136:LEU:HD23	1:A:149:GLN:O	1.99	0.61
1:B:7:LEU:HD13	1:B:15:VAL:HG21	1.82	0.61
1:A:38:LYS:HG3	1:A:44:CYS:C	2.27	0.60
1:A:45:PRO:HD2	2:A:713:HOH:O	2.00	0.60
1:B:132:VAL:HG13	1:B:174:VAL:HG12	1.84	0.60
1:A:66:GLN:NE2	1:A:77:LEU:H	2.00	0.59
1:A:140:HIS:O	1:A:141:ASP:HB2	2.03	0.58
1:A:40:GLY:HA3	2:A:529:HOH:O	2.04	0.58
1:B:156:ASP:OD2	1:B:160:ASN:HB2	2.04	0.58
1:A:26:HIS:NE2	1:A:127:HIS:CE1	2.72	0.57
1:A:130:ILE:HG22	1:A:132:VAL:HG23	1.85	0.57
1:A:103:PRO:HB2	1:A:165:VAL:HG23	1.86	0.57
1:B:68:LEU:N	1:B:68:LEU:HD23	2.19	0.57
1:A:20:THR:O	1:A:177:LYS:HD2	2.04	0.57
1:A:50:ARG:HG3	2:A:708:HOH:O	2.04	0.57
1:A:54:GLU:H	1:A:54:GLU:CD	2.13	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:HIS:C	1:A:127:HIS:HD2	2.13	0.56
1:B:17:THR:HG23	1:B:70:LEU:O	2.05	0.56
1:B:101:GLN:HE21	1:B:164:VAL:HG11	1.71	0.55
1:B:146:LYS:NZ	1:B:148:ASP:OD1	2.39	0.55
1:B:142:GLU:OE2	1:B:142:GLU:HA	2.05	0.55
1:A:127:HIS:NE2	1:A:130:ILE:CB	2.55	0.55
1:A:136:LEU:HD21	1:A:150:TYR:CE1	2.42	0.55
1:A:101:GLN:HG2	1:A:154:HIS:CD2	2.41	0.55
1:A:53:ASN:N	1:A:53:ASN:ND2	2.50	0.54
1:A:9:ASP:HB2	1:A:175:LEU:O	2.07	0.54
1:A:125:VAL:HG12	1:A:127:HIS:H	1.73	0.54
1:A:92:PRO:HG3	2:A:728:HOH:O	2.06	0.53
1:A:125:VAL:HG12	1:A:127:HIS:HB3	1.89	0.53
1:B:128:SER:HB2	1:B:130:ILE:CB	2.39	0.53
1:B:97:VAL:O	1:B:103:PRO:HA	2.09	0.52
1:B:127:HIS:O	1:B:128:SER:CB	2.57	0.52
1:B:85:PRO:HG3	1:B:92:PRO:HB3	1.91	0.52
1:A:6:ASP:HA	1:A:72:ILE:O	2.10	0.52
1:B:65:SER:HB2	1:B:72:ILE:HG12	1.92	0.52
1:B:146:LYS:HE2	1:B:148:ASP:CB	2.25	0.51
1:A:103:PRO:HB2	1:A:165:VAL:HG21	1.92	0.51
1:B:15:VAL:HG13	1:B:21:TYR:CE1	2.45	0.51
1:A:27:ILE:HB	1:A:30:HIS:CD2	2.44	0.51
1:A:55:VAL:HG13	1:A:56:SER:N	2.26	0.51
1:B:82:PHE:O	1:B:92:PRO:HB2	2.11	0.50
1:B:96:VAL:CG1	1:B:103:PRO:HB3	2.42	0.50
1:A:114:GLU:HB2	2:A:443:HOH:O	2.12	0.50
1:A:153:ILE:HG21	1:A:161:ARG:HG2	1.94	0.49
1:B:132:VAL:HG13	1:B:174:VAL:CG1	2.41	0.49
1:A:125:VAL:C	1:A:127:HIS:H	2.21	0.49
1:A:162:ARG:HB3	2:A:646:HOH:O	2.12	0.49
1:B:120:PHE:HB3	1:B:135:LEU:HD11	1.93	0.49
1:A:34:ILE:HD13	2:A:708:HOH:O	2.13	0.49
1:A:54:GLU:HG3	2:A:735:HOH:O	2.13	0.48
1:B:128:SER:C	1:B:130:ILE:N	2.66	0.48
1:B:62:ARG:HD2	2:B:721:HOH:O	2.13	0.47
1:B:101:GLN:NE2	1:B:164:VAL:HG11	2.29	0.47
1:B:142:GLU:CD	1:B:142:GLU:O	2.58	0.47
1:A:6:ASP:OD2	1:A:73:PRO:HA	2.15	0.46
1:B:86:PRO:HG3	2:B:497:HOH:O	2.14	0.46
1:B:128:SER:C	1:B:130:ILE:H	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:ARG:HG2	1:B:62:ARG:NH1	2.31	0.45
1:B:128:SER:HB2	1:B:130:ILE:H	1.80	0.45
1:B:128:SER:OG	1:B:132:VAL:HG23	2.16	0.45
1:B:128:SER:OG	1:B:132:VAL:CG2	2.65	0.45
1:A:115:LYS:HB3	2:A:706:HOH:O	2.16	0.45
1:A:7:LEU:HD11	1:A:122:PHE:CD2	2.52	0.45
1:B:42:GLU:CD	1:B:46:LEU:HB2	2.41	0.45
1:A:33:GLY:HA3	1:A:57:LYS:O	2.17	0.45
1:A:91:SER:N	2:A:609:HOH:O	2.49	0.44
1:A:39:THR:O	1:A:42:GLU:HG3	2.16	0.44
1:A:136:LEU:HD23	1:A:149:GLN:C	2.42	0.44
1:B:48:VAL:HG21	1:B:105:VAL:HG12	2.00	0.44
1:B:128:SER:HB2	1:B:130:ILE:HB	1.98	0.44
1:B:49:VAL:HG12	1:B:162:ARG:HA	1.99	0.44
1:B:115:LYS:HG3	2:B:461:HOH:O	2.18	0.44
1:A:49:VAL:HG12	1:A:162:ARG:HA	2.00	0.44
1:B:6:ASP:N	2:B:392:HOH:O	2.51	0.44
1:A:91:SER:HA	1:A:92:PRO:HD3	1.81	0.43
1:B:33:GLY:HA3	1:B:57:LYS:O	2.18	0.43
1:A:44:CYS:HB2	1:A:45:PRO:CD	2.49	0.43
1:B:8:VAL:HG22	1:B:12:GLY:C	2.44	0.43
1:B:59:GLU:HB3	2:B:705:HOH:O	2.18	0.43
1:A:23:LEU:CD2	1:A:175:LEU:HG	2.48	0.43
1:A:156:ASP:OD1	1:A:160:ASN:HB2	2.18	0.42
1:A:67:PHE:HE2	1:A:76:SER:HB3	1.84	0.42
1:B:33:GLY:HA3	1:B:57:LYS:C	2.44	0.42
1:A:22:TYR:CZ	1:A:57:LYS:HD3	2.54	0.42
1:B:104:ALA:HB1	2:B:396:HOH:O	2.19	0.42
1:B:146:LYS:NZ	1:B:148:ASP:HB3	2.35	0.42
1:B:146:LYS:HZ3	1:B:148:ASP:CG	2.26	0.42
1:B:127:HIS:C	1:B:128:SER:HG	2.28	0.42
1:A:86:PRO:O	1:A:87:SER:C	2.63	0.42
1:B:99:SER:OG	1:B:102:GLY:O	2.35	0.42
1:A:145:VAL:HG22	1:A:146:LYS:N	2.35	0.42
1:B:62:ARG:HG2	1:B:62:ARG:HH11	1.85	0.42
1:A:63:ILE:HG22	1:A:64:SER:N	2.34	0.41
1:A:132:VAL:HG22	1:A:174:VAL:HG12	2.02	0.41
1:A:139:GLN:HA	2:A:519:HOH:O	2.19	0.41
1:A:175:LEU:HD12	1:A:175:LEU:N	2.36	0.41
1:B:35:GLU:HB2	1:B:36:THR:H	1.75	0.41
1:B:7:LEU:HD23	1:B:7:LEU:HA	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:GLY:HA2	1:B:131:HIS:CE1	2.55	0.41
1:B:23:LEU:HB2	1:B:61:ILE:HD13	2.02	0.41
1:A:148:ASP:OD2	1:A:148:ASP:N	2.40	0.41
1:B:62:ARG:CD	2:B:721:HOH:O	2.68	0.41
1:A:16:GLU:H	1:A:21:TYR:HH	1.65	0.41
1:A:151:ILE:HG22	1:A:171:LEU:HD12	2.03	0.41
1:B:130:ILE:H	1:B:130:ILE:HG12	1.57	0.41
1:B:142:GLU:OE2	1:B:142:GLU:CA	2.69	0.41
1:A:124:LYS:HA	1:A:133:TYR:CD1	2.56	0.41
1:A:51:SER:HA	1:A:52:PRO:HD3	1.92	0.40
1:B:32:GLY:HA3	1:B:56:SER:O	2.21	0.40
1:A:50:ARG:HA	2:A:708:HOH:O	2.21	0.40
1:A:123:GLU:OE1	1:A:136:LEU:HD11	2.21	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	166/186 (89%)	152 (92%)	11 (7%)	3 (2%)	6	22
1	B	171/186 (92%)	154 (90%)	12 (7%)	5 (3%)	3	12
All	All	337/372 (91%)	306 (91%)	23 (7%)	8 (2%)	4	16

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	130	ILE
1	B	143	GLU
1	A	126	SER
1	B	128	SER
1	B	168	GLU

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Mol	Chain	Res	Type
1	A	87	SER
1	B	45	PRO
1	B	169	ASN

### 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	147/163 (90%)	135 (92%)	12 (8%)	10	31
1	B	151/163 (93%)	132 (87%)	19 (13%)	4	14
All	All	298/326 (91%)	267 (90%)	31 (10%)	7	21

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

Mol	Chain	Res	Type
1	A	41	ASN
1	A	53	ASN
1	A	115	LYS
1	A	118	LEU
1	A	126	SER
1	A	127	HIS
1	A	129	ASN
1	A	130	ILE
1	A	138	CYS
1	A	155	ARG
1	A	161	ARG
1	A	167	GLU
1	B	7	LEU
1	B	8	VAL
1	B	24	LEU
1	B	68	LEU
1	B	70	LEU
1	B	87	SER
1	B	110	GLN
1	B	112	LEU

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Mol	Chain	Res	Type
1	B	128	SER
1	B	130	ILE
1	B	132	VAL
1	B	141	ASP
1	B	142	GLU
1	B	143	GLU
1	B	144	ASP
1	B	145	VAL
1	B	167	GLU
1	B	170	PRO
1	B	177	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	30	HIS
1	A	53	ASN
1	A	66	GLN
1	A	127	HIS
1	A	158	ASN
1	B	30	HIS
1	B	66	GLN
1	B	101	GLN
1	B	110	GLN
1	B	131	HIS
1	B	140	HIS
1	B	154	HIS
1	B	160	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 oligosaccharides 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

### 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.