



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 09:05 am BST

PDB ID : 1YZE
Title : Crystal structure of the N-terminal domain of USP7/HAUSP.
Authors : Saridakis, V.; Sheng, Y.; Sarkari, F.; Holowaty, M.N.; Shire, K.; Nguyen, T.; Zhang, R.G.; Liao, J.; Lee, W.; Edwards, A.M.; Arrowsmith, C.H.; Frappier, L.
Deposited on : 2005-02-28
Resolution : 2.00 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

<https://www.wwpdb.org/validation/2017/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
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

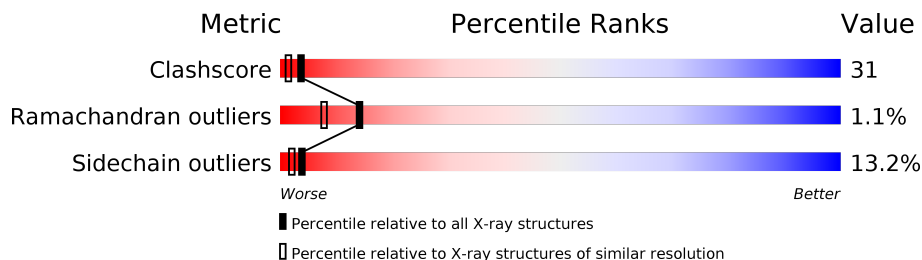
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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 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	155	27% 34% 35%
1	B	155	26% 32% 6% 36%
1	C	155	30% 29% 37%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2537 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 Ubiquitin carboxyl-terminal hydrolase 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	101	840	552	144	138	6	0	0	0
1	B	99	813	533	138	136	6	0	0	0
1	C	98	794	519	132	137	6	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	51	GLY	-	cloning artifact	UNP Q93009
A	52	SER	-	cloning artifact	UNP Q93009
A	53	HIS	-	cloning artifact	UNP Q93009
B	51	GLY	-	cloning artifact	UNP Q93009
B	52	SER	-	cloning artifact	UNP Q93009
B	53	HIS	-	cloning artifact	UNP Q93009
C	51	GLY	-	cloning artifact	UNP Q93009
C	52	SER	-	cloning artifact	UNP Q93009
C	53	HIS	-	cloning artifact	UNP Q93009

- Molecule 2 is water.

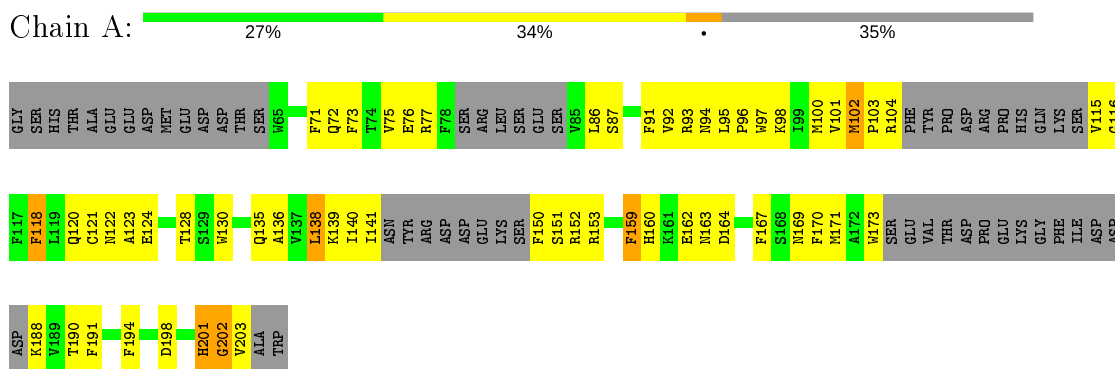
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	35	Total	O	0	0
			35	35		
2	B	25	Total	O	0	0
			25	25		
2	C	30	Total	O	0	0
			30	30		

3 Residue-property plots [i](#)

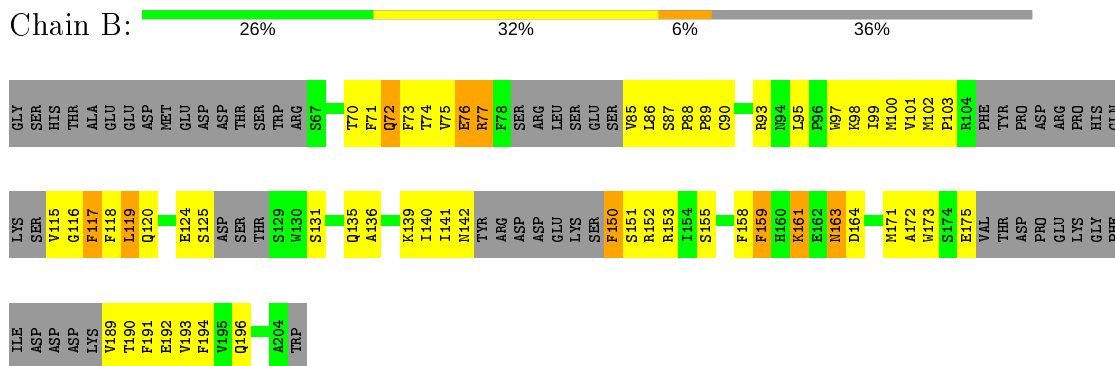
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

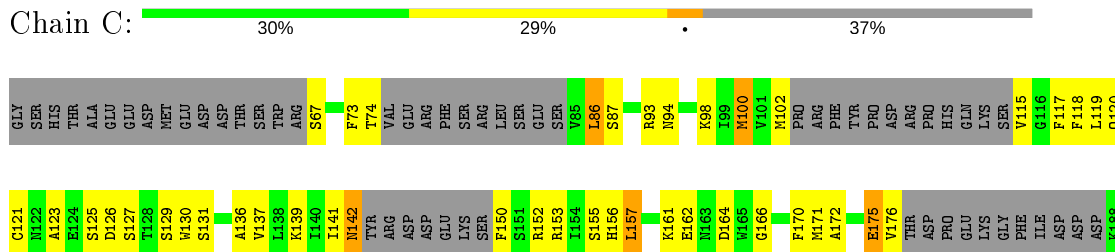
- Molecule 1: Ubiquitin carboxyl-terminal hydrolase 7



- Molecule 1: Ubiquitin carboxyl-terminal hydrolase 7



- Molecule 1: Ubiquitin carboxyl-terminal hydrolase 7



V189	P200
T190	H201
F191	G202
E192	V203
V193	A204
F194	TRP

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	102.61Å 102.61Å 45.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	26.96 – 2.00	Depositor
% Data completeness (in resolution range)	98.2 (26.96-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.325 , 0.367	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	2537	wwPDB-VP
Average B, all atoms (Å ²)	21.0	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	0.52	0/867	0.70	0/1170
1	B	0.52	0/837	0.67	0/1128
1	C	0.49	0/817	0.74	0/1103
All	All	0.51	0/2521	0.70	0/3401

There are no bond length outliers.

There are no bond angle outliers.

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	840	0	801	51	0
1	B	813	0	770	60	0
1	C	794	0	752	38	0
2	A	35	0	0	6	0
2	B	25	0	0	3	0
2	C	30	0	0	4	0
All	All	2537	0	2323	149	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 31.

All (149) 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:172:ALA:HB3	1:C:175:GLU:HB2	1.48	0.94
1:C:100:MET:HG2	1:C:118:PHE:HB2	1.54	0.89
1:B:151:SER:O	1:B:152:ARG:HG3	1.79	0.82
1:A:139:LYS:HD3	1:A:141:ILE:HD13	1.61	0.80
1:B:72:GLN:NE2	1:B:192:GLU:HG3	1.97	0.80
1:B:172:ALA:HB3	1:B:175:GLU:HG2	1.64	0.78
1:A:98:LYS:NZ	1:A:120:GLN:HE21	1.82	0.78
1:B:77:ARG:HH11	1:B:77:ARG:HG3	1.51	0.73
1:A:77:ARG:HD3	1:A:77:ARG:O	1.89	0.73
1:A:73:PHE:CG	1:A:87:SER:HB3	2.23	0.72
1:A:86:LEU:CD2	1:A:100:MET:HG2	2.20	0.72
1:A:139:LYS:HB2	1:A:151:SER:HB3	1.72	0.71
1:B:189:VAL:O	1:B:189:VAL:HG12	1.93	0.69
1:A:123:ALA:HB2	1:A:163:ASN:HD21	1.59	0.68
1:C:129:SER:O	1:C:202:GLY:HA3	1.94	0.67
1:C:172:ALA:HB3	1:C:175:GLU:CB	2.23	0.67
1:B:194:PHE:CZ	1:B:196:GLN:HG3	2.30	0.66
1:A:73:PHE:CD2	1:A:87:SER:HB3	2.30	0.66
1:B:103:PRO:HA	1:B:173:TRP:CZ3	2.30	0.66
1:B:71:PHE:CE1	1:B:99:ILE:HG13	2.30	0.66
1:A:75:VAL:HG21	1:A:101:VAL:HG21	1.76	0.65
1:B:72:GLN:HE22	1:B:192:GLU:HG3	1.59	0.65
1:C:152:ARG:HD3	1:C:170:PHE:CD2	2.31	0.64
1:A:86:LEU:HD23	1:A:100:MET:HG2	1.78	0.64
1:B:115:VAL:N	2:B:1004:HOH:O	2.30	0.63
1:B:99:ILE:HG23	1:B:117:PHE:CE1	2.33	0.63
1:A:152:ARG:HG3	1:A:170:PHE:CE2	2.34	0.63
1:C:67:SER:N	2:C:1038:HOH:O	2.32	0.62
1:C:141:ILE:O	1:C:142:ASN:HB3	1.98	0.62
1:A:140:ILE:HG12	1:A:191:PHE:CD1	2.36	0.61
1:B:76:GLU:HB2	1:B:77:ARG:NE	2.15	0.61
1:A:98:LYS:CE	1:A:120:GLN:HE21	2.14	0.60
1:B:74:THR:HA	1:B:190:THR:HG22	1.83	0.60
1:B:163:ASN:C	1:B:163:ASN:HD22	2.05	0.59
1:C:152:ARG:HD3	1:C:170:PHE:CE2	2.37	0.59
1:B:124:GLU:O	1:B:125:SER:HB2	2.01	0.58
1:A:103:PRO:O	1:A:104:ARG:HB2	2.03	0.58
1:B:136:ALA:O	1:B:153:ARG:HB2	2.03	0.58
1:B:100:MET:CE	1:B:120:GLN:HB2	2.34	0.58
1:B:101:VAL:HA	1:B:116:GLY:O	2.04	0.58
1:A:141:ILE:HG22	1:A:190:THR:HB	1.86	0.57
1:A:138:LEU:N	1:A:138:LEU:HD23	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:VAL:HG23	1:A:173:TRP:CZ3	2.40	0.57
1:B:100:MET:HE3	1:B:120:GLN:HB2	1.86	0.56
1:B:139:LYS:HA	1:B:150:PHE:O	2.04	0.56
1:A:72:GLN:OE1	1:A:190:THR:HG21	2.05	0.56
1:A:123:ALA:HB2	1:A:163:ASN:ND2	2.20	0.56
1:B:115:VAL:HA	1:B:173:TRP:CZ3	2.41	0.56
1:A:91:PHE:HA	1:A:95:LEU:O	2.06	0.55
1:C:150:PHE:HE1	1:C:170:PHE:O	1.89	0.55
1:C:190:THR:HG22	2:C:1081:HOH:O	2.07	0.55
1:A:201:HIS:N	1:A:201:HIS:CD2	2.75	0.54
1:A:153:ARG:HH11	1:A:153:ARG:HG3	1.71	0.54
1:C:127:SER:HG	1:C:130:TRP:HD1	1.53	0.54
1:C:150:PHE:CZ	1:C:152:ARG:HD2	2.43	0.54
1:A:102:MET:SD	1:A:118:PHE:HE1	2.30	0.54
1:B:73:PHE:CG	1:B:87:SER:HB2	2.43	0.54
1:A:76:GLU:OE1	1:A:188:LYS:HD2	2.09	0.53
1:B:173:TRP:HZ2	2:B:1048:HOH:O	1.91	0.52
1:B:76:GLU:O	1:B:77:ARG:HG2	2.10	0.52
1:C:150:PHE:CE1	1:C:152:ARG:HD2	2.45	0.52
1:C:203:VAL:O	1:C:204:ALA:CB	2.58	0.52
1:A:139:LYS:HE3	1:A:150:PHE:HD2	1.75	0.51
1:B:93:ARG:O	1:B:95:LEU:HD12	2.10	0.51
1:A:159:PHE:CE1	1:A:162:GLU:HB2	2.46	0.51
1:C:137:VAL:HG22	1:C:153:ARG:HG2	1.92	0.51
1:A:91:PHE:CZ	1:A:96:PRO:HB3	2.46	0.51
1:C:131:SER:HB2	1:C:157:LEU:HD21	1.93	0.51
1:A:115:VAL:HG23	1:A:173:TRP:HZ3	1.74	0.50
1:A:77:ARG:CD	1:A:77:ARG:O	2.59	0.50
1:C:86:LEU:HD12	1:C:98:LYS:HD3	1.93	0.50
1:B:117:PHE:CE2	1:B:191:PHE:HD1	2.29	0.50
1:B:172:ALA:HB3	1:B:175:GLU:CG	2.37	0.50
1:B:77:ARG:NH1	1:B:77:ARG:HG3	2.24	0.50
1:C:73:PHE:CD2	1:C:87:SER:HB3	2.47	0.50
1:B:73:PHE:CE1	1:B:88:PRO:HD3	2.47	0.50
1:A:130:TRP:HA	2:A:1003:HOH:O	2.11	0.49
1:C:93:ARG:HB3	1:C:200:PRO:HD3	1.94	0.49
1:C:136:ALA:HA	1:C:194:PHE:O	2.13	0.49
1:B:141:ILE:O	1:B:142:ASN:HB2	2.13	0.49
1:C:74:THR:OG1	1:C:190:THR:HB	2.13	0.48
1:B:120:GLN:HA	1:B:164:ASP:HA	1.94	0.48
1:C:100:MET:HG3	1:C:100:MET:O	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:ILE:HG12	1:B:193:VAL:HG21	1.94	0.48
1:B:99:ILE:HG12	1:B:193:VAL:CG2	2.44	0.48
1:A:124:GLU:HA	1:A:124:GLU:OE1	2.14	0.48
1:A:73:PHE:CG	1:A:87:SER:CB	2.95	0.48
1:A:98:LYS:HZ1	1:A:120:GLN:HE21	1.59	0.47
1:A:115:VAL:N	1:A:171:MET:O	2.47	0.47
1:B:119:LEU:O	1:B:164:ASP:HA	2.14	0.47
1:B:153:ARG:HH21	1:B:155:SER:HB2	1.78	0.47
1:B:140:ILE:HD12	1:B:171:MET:SD	2.55	0.47
1:C:120:GLN:HG2	1:C:121:CYS:N	2.29	0.47
1:B:140:ILE:O	1:B:150:PHE:CD2	2.68	0.47
1:C:171:MET:HG2	1:C:172:ALA:N	2.29	0.47
1:B:100:MET:HB2	2:B:1029:HOH:O	2.15	0.47
1:B:75:VAL:HG21	1:B:101:VAL:HG21	1.97	0.47
1:A:202:GLY:N	2:A:1003:HOH:O	2.48	0.47
1:B:131:SER:HA	1:B:158:PHE:O	2.14	0.47
1:B:76:GLU:HB2	1:B:77:ARG:HE	1.79	0.47
1:A:139:LYS:HB2	1:A:151:SER:CB	2.44	0.46
1:C:94:ASN:ND2	2:C:1068:HOH:O	2.48	0.46
1:C:127:SER:OG	1:C:130:TRP:HD1	1.98	0.46
1:C:156:HIS:HE1	1:C:162:GLU:O	1.99	0.46
1:A:198:ASP:HB2	2:A:1011:HOH:O	2.16	0.46
1:B:76:GLU:C	1:B:77:ARG:HG2	2.35	0.46
1:C:152:ARG:HB2	1:C:170:PHE:CE2	2.51	0.45
1:C:118:PHE:HA	1:C:166:GLY:HA3	1.98	0.45
1:A:97:TRP:HA	1:A:120:GLN:O	2.17	0.45
1:B:136:ALA:O	1:B:153:ARG:CB	2.64	0.45
1:B:87:SER:O	1:B:98:LYS:HD3	2.16	0.45
1:C:153:ARG:HG3	1:C:153:ARG:HH11	1.81	0.45
1:A:118:PHE:CD1	1:A:118:PHE:N	2.84	0.45
1:A:139:LYS:HG2	1:A:140:ILE:N	2.31	0.45
1:A:135:GLN:O	1:A:135:GLN:HG3	2.16	0.45
1:A:100:MET:SD	1:A:120:GLN:HB2	2.57	0.44
1:A:160:HIS:HB2	2:A:1089:HOH:O	2.16	0.44
1:B:115:VAL:N	1:B:173:TRP:HE3	2.15	0.44
1:A:116:GLY:HA2	1:A:167:PHE:O	2.18	0.44
1:B:100:MET:HB3	1:B:118:PHE:HB2	1.99	0.43
1:B:194:PHE:HZ	1:B:196:GLN:HG3	1.81	0.43
1:C:120:GLN:CD	1:C:123:ALA:HB3	2.39	0.43
1:B:86:LEU:CD2	1:B:100:MET:HG3	2.49	0.43
1:B:70:THR:HA	1:B:193:VAL:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:LYS:HD2	2:C:1082:HOH:O	2.18	0.43
1:B:86:LEU:HG	1:B:100:MET:HG3	2.01	0.43
1:C:171:MET:SD	1:C:176:VAL:HB	2.58	0.42
1:A:160:HIS:N	2:A:1089:HOH:O	2.47	0.42
1:B:115:VAL:HA	1:B:173:TRP:HZ3	1.83	0.42
1:A:159:PHE:HE1	1:A:162:GLU:HB2	1.82	0.42
1:C:139:LYS:HG2	1:C:192:GLU:HB3	2.02	0.42
1:A:201:HIS:C	2:A:1003:HOH:O	2.57	0.42
1:B:89:PRO:HB3	1:B:98:LYS:HE3	2.02	0.42
1:C:120:GLN:NE2	1:C:123:ALA:HB3	2.35	0.42
1:A:201:HIS:H	1:A:201:HIS:CD2	2.38	0.42
1:A:136:ALA:HA	1:A:194:PHE:O	2.20	0.42
1:C:120:GLN:CG	1:C:123:ALA:HB2	2.50	0.42
1:C:115:VAL:HB	1:C:171:MET:O	2.20	0.42
1:B:103:PRO:HB3	1:B:173:TRP:CH2	2.55	0.41
1:B:159:PHE:CZ	1:B:161:LYS:HB2	2.55	0.41
1:A:92:VAL:O	1:A:93:ARG:HB2	2.19	0.41
1:B:73:PHE:CD1	1:B:88:PRO:HD3	2.56	0.41
1:B:73:PHE:CD1	1:B:87:SER:HB2	2.56	0.41
1:C:119:LEU:HD13	1:C:193:VAL:HG11	2.02	0.41
1:B:77:ARG:HD3	1:B:77:ARG:N	2.36	0.41
1:A:121:CYS:O	1:A:163:ASN:HB2	2.21	0.41
1:B:77:ARG:CG	1:B:77:ARG:NH1	2.80	0.41
1:B:140:ILE:O	1:B:150:PHE:HD2	2.04	0.40
1:B:90:CYS:O	1:B:97:TRP:N	2.50	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	91/155 (59%)	82 (90%)	8 (9%)	1 (1%)	14 8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	87/155 (56%)	81 (93%)	5 (6%)	1 (1%)	14	8
1	C	88/155 (57%)	81 (92%)	6 (7%)	1 (1%)	14	8
All	All	266/465 (57%)	244 (92%)	19 (7%)	3 (1%)	14	8

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	125	SER
1	B	161	LYS
1	A	202	GLY

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	91/141 (64%)	79 (87%)	12 (13%)	4	2
1	B	88/141 (62%)	77 (88%)	11 (12%)	4	2
1	C	87/141 (62%)	75 (86%)	12 (14%)	3	2
All	All	266/423 (63%)	231 (87%)	35 (13%)	4	2

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	PHE
1	A	94	ASN
1	A	102	MET
1	A	118	PHE
1	A	122	ASN
1	A	128	THR
1	A	138	LEU
1	A	159	PHE
1	A	164	ASP
1	A	169	ASN
1	A	201	HIS

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Mol	Chain	Res	Type
1	A	203	VAL
1	B	72	GLN
1	B	76	GLU
1	B	77	ARG
1	B	85	VAL
1	B	102	MET
1	B	117	PHE
1	B	119	LEU
1	B	135	GLN
1	B	150	PHE
1	B	159	PHE
1	B	163	ASN
1	C	86	LEU
1	C	100	MET
1	C	102	MET
1	C	117	PHE
1	C	126	ASP
1	C	142	ASN
1	C	155	SER
1	C	157	LEU
1	C	161	LYS
1	C	164	ASP
1	C	175	GLU
1	C	190	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	GLN
1	A	122	ASN
1	A	135	GLN
1	A	163	ASN
1	A	169	ASN
1	A	201	HIS
1	B	72	GLN
1	B	160	HIS
1	B	163	ASN
1	B	169	ASN
1	B	196	GLN
1	C	72	GLN
1	C	94	ASN
1	C	120	GLN

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Mol	Chain	Res	Type
1	C	156	HIS
1	C	169	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 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

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.