



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:26 PM GMT

PDB ID : 1ATU
Title : UNCLEAVED ALPHA-1-ANTITRYPSIN
Authors : Ryu, S.-E.; Choi, H.-J.
Deposited on : 1997-05-11
Resolution : 2.70 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

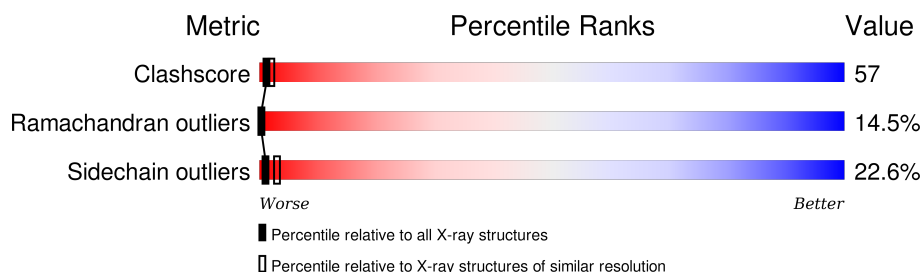
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)

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	374	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2962 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 ALPHA-1-ANTITRYPSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	374	Total	C	N	O	S	0	0	0
			2962	1908	486	559	9			

There are 7 discrepancies between the modelled and reference sequences:

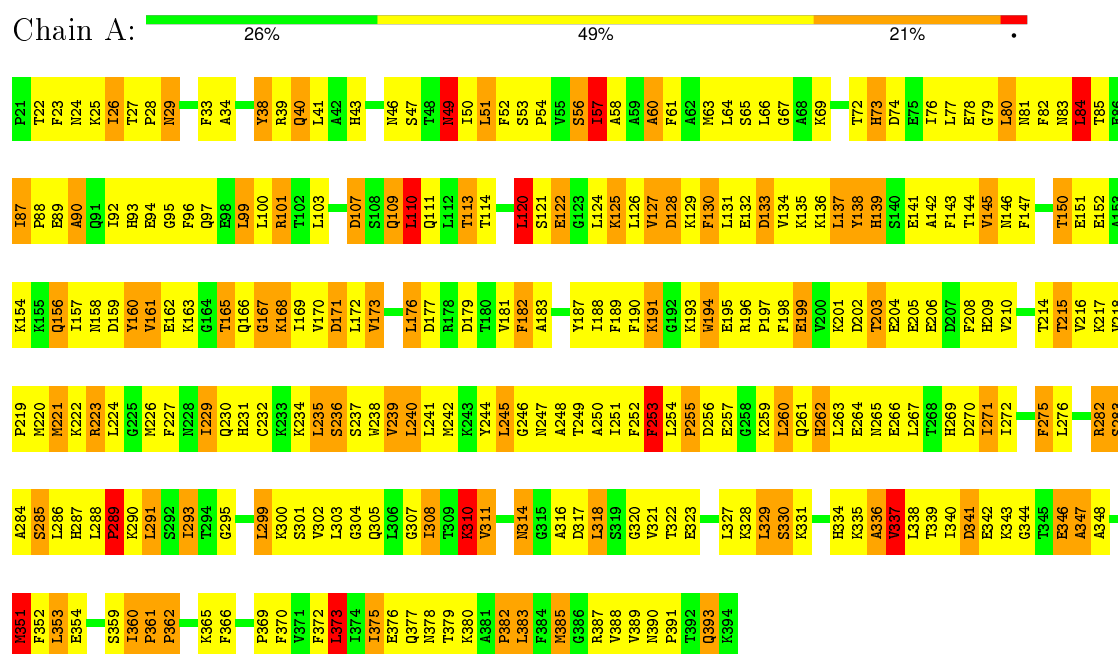
Chain	Residue	Modelled	Actual	Comment	Reference
A	51	LEU	PHE	ENGINEERED	UNP P01009
A	59	ALA	THR	ENGINEERED	UNP P01009
A	68	ALA	THR	ENGINEERED	UNP P01009
A	70	GLY	ALA	ENGINEERED	UNP P01009
A	374	ILE	MET	ENGINEERED	UNP P01009
A	381	ALA	SER	ENGINEERED	UNP P01009
A	387	ARG	LYS	ENGINEERED	UNP P01009

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: ALPHA-1-ANTITRYPSIN



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	115.78Å 39.37Å 90.43Å 90.00° 103.80° 90.00°	Depositor
Resolution (Å)	8.00 – 2.70	Depositor
% Data completeness (in resolution range)	83.5 (8.00-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.195 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2962	wwPDB-VP
Average B, all atoms (Å ²)	11.0	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	0.61	0/3023	0.87	5/4086 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	351	MET	N-CA-C	-6.04	94.68	111.00
1	A	49	ASN	N-CA-C	-5.37	96.49	111.00
1	A	137	LEU	CA-CB-CG	5.08	126.97	115.30
1	A	347	ALA	N-CA-C	5.02	124.55	111.00
1	A	353	LEU	CA-CB-CG	5.00	126.81	115.30

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	2962	0	2988	337	0
All	All	2962	0	2988	337	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 57.

All (337) 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:360:ILE:HB	1:A:361:PRO:HD3	1.27	1.11
1:A:128:ASP:HB2	1:A:132:GLU:HB2	1.32	1.10
1:A:161:VAL:HG12	1:A:187:TYR:HB3	1.30	1.08
1:A:76:ILE:HD12	1:A:308:ILE:HG23	1.35	1.05
1:A:240:LEU:HD11	1:A:286:LEU:HD11	1.33	1.04
1:A:359:SER:HB2	1:A:362:PRO:HG3	1.37	1.04
1:A:359:SER:HB2	1:A:362:PRO:CG	1.93	0.98
1:A:219:PRO:HB2	1:A:290:LYS:HB3	1.43	0.97
1:A:311:VAL:HG13	1:A:318:LEU:HG	1.49	0.94
1:A:22:THR:HG21	1:A:95:GLY:HA2	1.50	0.94
1:A:235:LEU:HD22	1:A:253:PHE:HZ	1.34	0.90
1:A:151:GLU:HA	1:A:154:LYS:HE2	1.53	0.89
1:A:251:ILE:HD13	1:A:272:ILE:HG21	1.59	0.85
1:A:131:LEU:HD11	1:A:142:ALA:HB2	1.59	0.85
1:A:224:LEU:HG	1:A:285:SER:HB3	1.57	0.83
1:A:287:HIS:HB3	1:A:365:LYS:HA	1.62	0.81
1:A:244:TYR:CZ	1:A:250:ALA:HB2	2.15	0.81
1:A:198:PHE:HZ	1:A:286:LEU:HD23	1.48	0.79
1:A:67:GLY:HA3	1:A:130:PHE:HA	1.63	0.79
1:A:239:VAL:O	1:A:240:LEU:HB2	1.81	0.78
1:A:130:PHE:HB3	1:A:320:GLY:HA3	1.64	0.78
1:A:96:PHE:HA	1:A:99:LEU:HB3	1.66	0.78
1:A:194:TRP:HA	1:A:244:TYR:HA	1.64	0.77
1:A:183:ALA:HB2	1:A:330:SER:HB2	1.65	0.76
1:A:121:SER:HA	1:A:145:VAL:O	1.86	0.76
1:A:194:TRP:O	1:A:245:LEU:HG	1.85	0.76
1:A:235:LEU:HD22	1:A:253:PHE:CZ	2.19	0.76
1:A:67:GLY:HA2	1:A:133:ASP:HB3	1.67	0.76
1:A:66:LEU:HD13	1:A:134:VAL:HA	1.66	0.76
1:A:103:LEU:HA	1:A:378:ASN:HB3	1.68	0.76
1:A:198:PHE:CZ	1:A:286:LEU:HD23	2.21	0.75
1:A:141:GLU:HG2	1:A:143:PHE:HE1	1.52	0.74
1:A:351:MET:O	1:A:351:MET:HG2	1.88	0.73
1:A:182:PHE:HE2	1:A:327:LEU:HD13	1.52	0.73
1:A:310:LYS:HG2	1:A:316:ALA:HB3	1.70	0.73
1:A:87:ILE:HG12	1:A:92:ILE:HD11	1.71	0.73
1:A:198:PHE:CZ	1:A:288:LEU:HD12	2.24	0.72
1:A:158:ASN:OD1	1:A:173:VAL:HG12	1.89	0.72
1:A:66:LEU:HB3	1:A:133:ASP:O	1.90	0.72
1:A:101:ARG:NH2	1:A:137:LEU:HD11	2.04	0.72
1:A:51:LEU:HB3	1:A:295:GLY:HA3	1.72	0.71
1:A:241:LEU:CD2	1:A:251:ILE:HG12	2.21	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:CYS:SG	1:A:235:LEU:HD11	2.31	0.71
1:A:232:CYS:SG	1:A:235:LEU:CD1	2.80	0.69
1:A:172:LEU:HD21	1:A:335:LYS:HG2	1.75	0.69
1:A:125:LYS:NZ	1:A:125:LYS:HA	2.07	0.69
1:A:314:ASN:HA	1:A:328:LYS:HD2	1.75	0.69
1:A:251:ILE:O	1:A:372:PHE:HB2	1.93	0.68
1:A:360:ILE:CB	1:A:361:PRO:HD3	2.16	0.68
1:A:60:ALA:HA	1:A:63:MET:SD	2.33	0.68
1:A:360:ILE:HB	1:A:361:PRO:CD	2.15	0.68
1:A:390:ASN:O	1:A:393:GLN:HG2	1.94	0.68
1:A:360:ILE:C	1:A:362:PRO:HD3	2.13	0.68
1:A:63:MET:O	1:A:66:LEU:HB2	1.93	0.67
1:A:195:GLU:O	1:A:197:PRO:HD3	1.94	0.67
1:A:241:LEU:HD21	1:A:251:ILE:HG12	1.77	0.67
1:A:165:THR:HG23	1:A:168:LYS:N	2.09	0.67
1:A:103:LEU:HB2	1:A:379:THR:HG23	1.76	0.67
1:A:34:ALA:HB2	1:A:54:PRO:HB3	1.77	0.67
1:A:128:ASP:HB2	1:A:132:GLU:CB	2.20	0.67
1:A:244:TYR:HB2	1:A:248:ALA:HB3	1.77	0.66
1:A:224:LEU:HG	1:A:285:SER:CB	2.26	0.66
1:A:240:LEU:HD11	1:A:286:LEU:CD1	2.20	0.66
1:A:67:GLY:CA	1:A:133:ASP:HB3	2.25	0.66
1:A:109:GLN:HB3	1:A:246:GLY:HA3	1.78	0.66
1:A:138:TYR:N	1:A:138:TYR:CD1	2.63	0.65
1:A:101:ARG:HH21	1:A:137:LEU:HD11	1.61	0.65
1:A:284:ALA:HA	1:A:362:PRO:HB3	1.79	0.64
1:A:299:LEU:HG	1:A:334:HIS:HD2	1.61	0.64
1:A:34:ALA:HB1	1:A:52:PHE:CZ	2.33	0.64
1:A:80:LEU:HB2	1:A:82:PHE:CD1	2.33	0.63
1:A:285:SER:H	1:A:362:PRO:HB3	1.63	0.63
1:A:204:GLU:O	1:A:220:MET:HB2	1.99	0.63
1:A:224:LEU:HG	1:A:285:SER:HA	1.79	0.63
1:A:161:VAL:O	1:A:165:THR:HB	1.99	0.63
1:A:161:VAL:HG12	1:A:187:TYR:CB	2.19	0.62
1:A:38:TYR:HA	1:A:41:LEU:HB3	1.82	0.62
1:A:346:GLU:O	1:A:348:ALA:N	2.33	0.62
1:A:237:SER:HB3	1:A:254:LEU:O	1.99	0.62
1:A:152:GLU:O	1:A:156:GLN:HB2	2.00	0.61
1:A:284:ALA:HB1	1:A:362:PRO:HA	1.83	0.61
1:A:251:ILE:HD12	1:A:375:ILE:HD11	1.81	0.61
1:A:318:LEU:HD12	1:A:328:LYS:C	2.20	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:ILE:O	1:A:362:PRO:HD3	2.00	0.61
1:A:67:GLY:O	1:A:69:LYS:HG3	2.01	0.60
1:A:141:GLU:HG2	1:A:143:PHE:CE1	2.35	0.60
1:A:232:CYS:HB2	1:A:235:LEU:HD11	1.81	0.60
1:A:143:PHE:O	1:A:144:THR:HG23	2.02	0.60
1:A:114:THR:HB	1:A:188:ILE:HD12	1.84	0.60
1:A:67:GLY:CA	1:A:130:PHE:HA	2.31	0.60
1:A:251:ILE:HG21	1:A:272:ILE:HD13	1.84	0.59
1:A:56:SER:OG	1:A:114:THR:HG21	2.02	0.59
1:A:376:GLU:O	1:A:380:LYS:HA	2.03	0.59
1:A:165:THR:O	1:A:168:LYS:HG2	2.03	0.59
1:A:241:LEU:HD23	1:A:250:ALA:O	2.03	0.59
1:A:311:VAL:HG11	1:A:329:LEU:HD12	1.84	0.58
1:A:40:GLN:HG3	1:A:302:VAL:HG12	1.86	0.58
1:A:182:PHE:CE2	1:A:327:LEU:HD13	2.36	0.58
1:A:201:LYS:HD2	1:A:201:LYS:N	2.19	0.58
1:A:289:PRO:HD3	1:A:366:PHE:CB	2.34	0.57
1:A:22:THR:HB	1:A:26:ILE:HG22	1.84	0.57
1:A:335:LYS:HD2	1:A:336:ALA:H	1.69	0.57
1:A:339:THR:C	1:A:340:ILE:HD12	2.24	0.57
1:A:131:LEU:HD22	1:A:321:VAL:HG13	1.86	0.57
1:A:223:ARG:HD3	1:A:227:PHE:HZ	1.70	0.57
1:A:161:VAL:CG1	1:A:187:TYR:HB3	2.21	0.57
1:A:310:LYS:HG2	1:A:316:ALA:CB	2.35	0.56
1:A:103:LEU:HD12	1:A:379:THR:HG21	1.87	0.56
1:A:78:GLU:HA	1:A:82:PHE:HB2	1.87	0.56
1:A:22:THR:HB	1:A:26:ILE:CG2	2.36	0.56
1:A:23:PHE:HA	1:A:27:THR:OG1	2.05	0.56
1:A:389:VAL:O	1:A:391:PRO:HD3	2.05	0.56
1:A:232:CYS:SG	1:A:235:LEU:HD13	2.46	0.56
1:A:216:VAL:HG12	1:A:218:VAL:HG23	1.88	0.56
1:A:154:LYS:O	1:A:158:ASN:ND2	2.39	0.56
1:A:187:TYR:HA	1:A:335:LYS:HB2	1.88	0.55
1:A:80:LEU:HB2	1:A:82:PHE:CE1	2.41	0.55
1:A:244:TYR:CE1	1:A:250:ALA:HB2	2.41	0.55
1:A:109:GLN:O	1:A:110:LEU:HB2	2.06	0.55
1:A:126:LEU:HD22	1:A:321:VAL:HG12	1.88	0.55
1:A:131:LEU:HD11	1:A:142:ALA:CB	2.34	0.55
1:A:373:LEU:HB3	1:A:385:MET:HG2	1.89	0.55
1:A:311:VAL:CG1	1:A:329:LEU:HD12	2.36	0.55
1:A:78:GLU:OE2	1:A:84:LEU:HD22	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:LEU:HD22	1:A:321:VAL:CG1	2.36	0.55
1:A:199:GLU:CB	1:A:202:ASP:HB3	2.36	0.54
1:A:287:HIS:CD2	1:A:365:LYS:HG3	2.42	0.54
1:A:161:VAL:HG21	1:A:172:LEU:HG	1.89	0.54
1:A:113:THR:O	1:A:188:ILE:HD12	2.07	0.54
1:A:283:SER:HB2	1:A:359:SER:HA	1.89	0.54
1:A:224:LEU:HG	1:A:285:SER:CA	2.38	0.54
1:A:340:ILE:HD12	1:A:340:ILE:N	2.23	0.54
1:A:114:THR:HB	1:A:188:ILE:CD1	2.37	0.54
1:A:299:LEU:HG	1:A:334:HIS:CD2	2.43	0.54
1:A:172:LEU:HD21	1:A:335:LYS:CG	2.38	0.53
1:A:223:ARG:HH11	1:A:227:PHE:HZ	1.55	0.53
1:A:240:LEU:HG	1:A:242:MET:SD	2.48	0.53
1:A:229:ILE:HD11	1:A:238:TRP:HE3	1.73	0.53
1:A:231:HIS:HD2	1:A:238:TRP:CD2	2.27	0.53
1:A:311:VAL:HG12	1:A:329:LEU:HB2	1.90	0.53
1:A:194:TRP:CZ2	1:A:341:ASP:O	2.62	0.53
1:A:230:GLN:HA	1:A:230:GLN:OE1	2.09	0.52
1:A:351:MET:HG3	1:A:354:GLU:HB2	1.91	0.52
1:A:222:LYS:HB2	1:A:287:HIS:ND1	2.24	0.52
1:A:78:GLU:HG2	1:A:84:LEU:HD13	1.91	0.52
1:A:137:LEU:HD12	1:A:138:TYR:CD1	2.45	0.52
1:A:138:TYR:N	1:A:138:TYR:HD1	2.07	0.52
1:A:54:PRO:HD2	1:A:382:PRO:O	2.10	0.52
1:A:232:CYS:CB	1:A:235:LEU:HD11	2.39	0.52
1:A:38:TYR:HD2	1:A:52:PHE:HE2	1.57	0.52
1:A:87:ILE:O	1:A:87:ILE:HG12	2.08	0.52
1:A:199:GLU:HG2	1:A:202:ASP:HB3	1.91	0.52
1:A:336:ALA:O	1:A:337:VAL:HG13	2.10	0.52
1:A:257:GLU:O	1:A:259:LYS:HG3	2.10	0.52
1:A:370:PHE:HE1	1:A:372:PHE:CD2	2.27	0.52
1:A:111:GLN:HE22	1:A:191:LYS:H	1.58	0.52
1:A:168:LYS:N	1:A:168:LYS:HE2	2.25	0.51
1:A:103:LEU:HB2	1:A:379:THR:CG2	2.40	0.51
1:A:226:MET:HA	1:A:282:ARG:O	2.10	0.51
1:A:289:PRO:HD3	1:A:366:PHE:HB2	1.92	0.51
1:A:314:ASN:HD22	1:A:328:LYS:NZ	2.09	0.51
1:A:160:TYR:C	1:A:162:GLU:H	2.14	0.51
1:A:137:LEU:HD12	1:A:138:TYR:HD1	1.74	0.51
1:A:275:PHE:N	1:A:275:PHE:HD1	2.08	0.51
1:A:69:LYS:HA	1:A:73:HIS:HB2	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:ALA:HB1	1:A:52:PHE:HZ	1.75	0.51
1:A:87:ILE:CG1	1:A:92:ILE:HD11	2.40	0.50
1:A:53:SER:O	1:A:57:ILE:HB	2.12	0.50
1:A:303:LEU:N	1:A:303:LEU:HD22	2.25	0.50
1:A:46:ASN:OD1	1:A:47:SER:N	2.45	0.50
1:A:65:SER:O	1:A:73:HIS:CD2	2.65	0.50
1:A:72:THR:O	1:A:74:ASP:N	2.45	0.50
1:A:393:GLN:O	1:A:393:GLN:HG3	2.12	0.49
1:A:351:MET:O	1:A:351:MET:CG	2.58	0.49
1:A:275:PHE:N	1:A:275:PHE:CD1	2.79	0.49
1:A:122:GLU:HB3	1:A:144:THR:O	2.12	0.49
1:A:29:ASN:ND2	1:A:81:ASN:HB2	2.26	0.49
1:A:361:PRO:N	1:A:362:PRO:HD3	2.23	0.49
1:A:276:LEU:HD13	1:A:380:LYS:HE3	1.95	0.49
1:A:66:LEU:HG	1:A:93:HIS:CE1	2.47	0.49
1:A:310:LYS:HE2	1:A:316:ALA:CB	2.43	0.49
1:A:33:PHE:CE1	1:A:80:LEU:HD22	2.47	0.49
1:A:194:TRP:HA	1:A:244:TYR:CA	2.37	0.49
1:A:127:VAL:N	1:A:322:THR:HA	2.28	0.49
1:A:375:ILE:HG22	1:A:380:LYS:C	2.32	0.49
1:A:288:LEU:HA	1:A:366:PHE:HB2	1.95	0.49
1:A:260:LEU:HD12	1:A:261:GLN:HG3	1.94	0.49
1:A:262:HIS:N	1:A:265:ASN:OD1	2.46	0.48
1:A:252:PHE:HA	1:A:372:PHE:HB3	1.96	0.48
1:A:49:ASN:HB2	1:A:393:GLN:OE1	2.14	0.48
1:A:165:THR:C	1:A:167:GLY:H	2.17	0.48
1:A:38:TYR:HD2	1:A:52:PHE:CE2	2.32	0.48
1:A:181:VAL:HG21	1:A:328:LYS:H	1.79	0.48
1:A:127:VAL:H	1:A:322:THR:HA	1.79	0.48
1:A:253:PHE:CG	1:A:263:LEU:HD12	2.49	0.47
1:A:160:TYR:O	1:A:163:LYS:HG2	2.13	0.47
1:A:322:THR:OG1	1:A:323:GLU:N	2.43	0.47
1:A:323:GLU:O	1:A:323:GLU:HG2	2.14	0.47
1:A:169:ILE:HG22	1:A:335:LYS:HE2	1.95	0.47
1:A:187:TYR:HA	1:A:335:LYS:CB	2.44	0.47
1:A:109:GLN:NE2	1:A:245:LEU:O	2.48	0.47
1:A:124:LEU:O	1:A:125:LYS:HG2	2.14	0.47
1:A:130:PHE:HB3	1:A:320:GLY:CA	2.40	0.47
1:A:132:GLU:HA	1:A:135:LYS:HG2	1.96	0.47
1:A:222:LYS:CG	1:A:223:ARG:N	2.77	0.47
1:A:50:ILE:HG22	1:A:51:LEU:N	2.30	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:GLU:HA	1:A:135:LYS:CG	2.45	0.47
1:A:314:ASN:ND2	1:A:328:LYS:HZ2	2.12	0.47
1:A:63:MET:O	1:A:134:VAL:HG22	2.15	0.47
1:A:34:ALA:HB2	1:A:54:PRO:CB	2.44	0.47
1:A:199:GLU:HG2	1:A:202:ASP:CB	2.45	0.47
1:A:158:ASN:O	1:A:161:VAL:HG23	2.14	0.47
1:A:190:PHE:HD2	1:A:338:LEU:CD1	2.28	0.47
1:A:83:ASN:O	1:A:87:ILE:HG23	2.15	0.47
1:A:84:LEU:HD13	1:A:84:LEU:H	1.79	0.47
1:A:302:VAL:HG23	1:A:303:LEU:HD22	1.96	0.47
1:A:157:ILE:CG2	1:A:158:ASN:N	2.78	0.46
1:A:235:LEU:HB2	1:A:263:LEU:HA	1.97	0.46
1:A:107:ASP:C	1:A:109:GLN:H	2.19	0.46
1:A:291:LEU:HD21	1:A:388:VAL:HG21	1.97	0.46
1:A:125:LYS:HZ3	1:A:125:LYS:HA	1.80	0.46
1:A:56:SER:O	1:A:57:ILE:HG13	2.14	0.46
1:A:159:ASP:O	1:A:162:GLU:HB3	2.15	0.46
1:A:373:LEU:HD12	1:A:382:PRO:HB3	1.96	0.46
1:A:125:LYS:CE	1:A:125:LYS:HA	2.46	0.46
1:A:38:TYR:C	1:A:40:GLN:H	2.19	0.46
1:A:199:GLU:HB3	1:A:202:ASP:HB3	1.98	0.46
1:A:314:ASN:ND2	1:A:328:LYS:NZ	2.64	0.45
1:A:272:ILE:O	1:A:272:ILE:HG22	2.16	0.45
1:A:109:GLN:HE21	1:A:109:GLN:HA	1.81	0.45
1:A:300:LYS:O	1:A:302:VAL:N	2.49	0.45
1:A:252:PHE:O	1:A:253:PHE:HB2	2.16	0.45
1:A:310:LYS:HE2	1:A:316:ALA:HB2	1.97	0.45
1:A:80:LEU:HB2	1:A:82:PHE:HD1	1.78	0.45
1:A:209:HIS:O	1:A:369:PRO:HD3	2.17	0.45
1:A:22:THR:C	1:A:24:ASN:H	2.20	0.45
1:A:130:PHE:O	1:A:134:VAL:HG23	2.15	0.45
1:A:373:LEU:CB	1:A:385:MET:HG2	2.47	0.45
1:A:163:LYS:HB2	1:A:163:LYS:HE3	1.81	0.45
1:A:34:ALA:HB1	1:A:54:PRO:HG3	1.98	0.45
1:A:338:LEU:HD12	1:A:339:THR:H	1.81	0.45
1:A:284:ALA:CA	1:A:362:PRO:HB3	2.45	0.45
1:A:135:LYS:O	1:A:136:LYS:C	2.55	0.45
1:A:165:THR:OG1	1:A:168:LYS:HB2	2.18	0.44
1:A:172:LEU:HD11	1:A:335:LYS:HG2	1.99	0.44
1:A:204:GLU:O	1:A:206:GLU:HG2	2.17	0.44
1:A:38:TYR:HA	1:A:41:LEU:CB	2.46	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:HIS:O	1:A:271:ILE:N	2.49	0.44
1:A:110:LEU:CD2	1:A:111:GLN:H	2.30	0.44
1:A:238:TRP:HZ3	1:A:282:ARG:NH2	2.15	0.44
1:A:254:LEU:HD12	1:A:370:PHE:HB3	1.99	0.44
1:A:142:ALA:C	1:A:143:PHE:HD1	2.20	0.44
1:A:120:LEU:HA	1:A:182:PHE:HB2	1.99	0.44
1:A:77:LEU:O	1:A:80:LEU:HG	2.17	0.44
1:A:208:PHE:CZ	1:A:369:PRO:HG3	2.53	0.44
1:A:137:LEU:HB3	1:A:138:TYR:CD1	2.53	0.44
1:A:137:LEU:HD13	1:A:137:LEU:C	2.38	0.44
1:A:172:LEU:CD2	1:A:335:LYS:HG2	2.47	0.43
1:A:79:GLY:C	1:A:81:ASN:H	2.20	0.43
1:A:150:THR:HG22	1:A:176:LEU:HD22	1.98	0.43
1:A:109:GLN:O	1:A:110:LEU:CB	2.65	0.43
1:A:359:SER:CB	1:A:362:PRO:HG3	2.28	0.43
1:A:222:LYS:HG3	1:A:223:ARG:N	2.34	0.43
1:A:260:LEU:O	1:A:263:LEU:HD23	2.18	0.43
1:A:291:LEU:HD22	1:A:340:ILE:HD13	1.99	0.43
1:A:131:LEU:HB2	1:A:321:VAL:HG13	2.00	0.43
1:A:236:SER:OG	1:A:262:HIS:HD2	2.02	0.43
1:A:157:ILE:HG23	1:A:158:ASN:N	2.32	0.43
1:A:287:HIS:O	1:A:366:PHE:HD1	2.01	0.43
1:A:216:VAL:HG11	1:A:391:PRO:HD2	1.99	0.43
1:A:57:ILE:HG22	1:A:58:ALA:N	2.32	0.43
1:A:103:LEU:CB	1:A:379:THR:HG23	2.45	0.43
1:A:127:VAL:HG23	1:A:322:THR:C	2.38	0.43
1:A:291:LEU:O	1:A:340:ILE:HB	2.18	0.43
1:A:168:LYS:HB3	1:A:337:VAL:HG21	2.00	0.43
1:A:218:VAL:HG12	1:A:219:PRO:O	2.18	0.43
1:A:237:SER:OG	1:A:255:PRO:HA	2.19	0.43
1:A:130:PHE:CE2	1:A:321:VAL:HG22	2.54	0.43
1:A:194:TRP:HA	1:A:245:LEU:H	1.84	0.42
1:A:135:LYS:HA	1:A:139:HIS:HA	2.01	0.42
1:A:318:LEU:HD13	1:A:318:LEU:O	2.19	0.42
1:A:340:ILE:O	1:A:341:ASP:HB3	2.18	0.42
1:A:72:THR:C	1:A:74:ASP:H	2.23	0.42
1:A:72:THR:C	1:A:74:ASP:N	2.72	0.42
1:A:170:VAL:O	1:A:172:LEU:N	2.52	0.42
1:A:203:THR:HG22	1:A:220:MET:O	2.20	0.42
1:A:328:LYS:HB2	1:A:328:LYS:HE3	1.67	0.42
1:A:103:LEU:HD12	1:A:379:THR:CG2	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:ILE:HD11	1:A:334:HIS:CE1	2.54	0.42
1:A:247:ASN:HA	1:A:377:GLN:NE2	2.35	0.42
1:A:253:PHE:HB3	1:A:263:LEU:HD12	2.01	0.42
1:A:244:TYR:CD2	1:A:248:ALA:HB3	2.55	0.42
1:A:114:THR:HB	1:A:188:ILE:HA	2.01	0.42
1:A:220:MET:SD	1:A:287:HIS:CD2	3.13	0.42
1:A:218:VAL:HG22	1:A:391:PRO:HG2	2.02	0.42
1:A:237:SER:HG	1:A:255:PRO:HA	1.85	0.42
1:A:263:LEU:HD23	1:A:263:LEU:H	1.85	0.42
1:A:87:ILE:CD1	1:A:92:ILE:HD11	2.50	0.42
1:A:196:ARG:NE	1:A:196:ARG:HA	2.35	0.42
1:A:122:GLU:HG3	1:A:146:ASN:ND2	2.35	0.41
1:A:27:THR:HB	1:A:28:PRO:HD3	2.02	0.41
1:A:147:PHE:CE2	1:A:182:PHE:HA	2.55	0.41
1:A:82:PHE:HD2	1:A:87:ILE:HD11	1.85	0.41
1:A:53:SER:HA	1:A:54:PRO:HD3	1.91	0.41
1:A:199:GLU:CG	1:A:202:ASP:HB3	2.49	0.41
1:A:172:LEU:HD21	1:A:335:LYS:HD3	2.01	0.41
1:A:304:GLY:HA2	1:A:308:ILE:O	2.20	0.41
1:A:239:VAL:HG12	1:A:240:LEU:H	1.84	0.41
1:A:221:MET:HG3	1:A:288:LEU:O	2.20	0.41
1:A:165:THR:HG23	1:A:168:LYS:H	1.82	0.41
1:A:254:LEU:HA	1:A:255:PRO:HD3	1.88	0.41
1:A:272:ILE:HG22	1:A:276:LEU:HG	2.02	0.41
1:A:266:GLU:O	1:A:267:LEU:HG	2.20	0.41
1:A:215:THR:O	1:A:217:LYS:HD2	2.20	0.41
1:A:227:PHE:HB3	1:A:242:MET:CE	2.51	0.41
1:A:220:MET:HB3	1:A:287:HIS:HE2	1.86	0.41
1:A:34:ALA:HB1	1:A:52:PHE:CE1	2.55	0.41
1:A:88:PRO:O	1:A:90:ALA:N	2.53	0.41
1:A:359:SER:HB2	1:A:362:PRO:HG2	1.94	0.41
1:A:223:ARG:NH2	1:A:353:LEU:O	2.54	0.41
1:A:370:PHE:CE1	1:A:372:PHE:HD2	2.38	0.41
1:A:83:ASN:O	1:A:85:THR:N	2.54	0.41
1:A:124:LEU:O	1:A:125:LYS:HE2	2.20	0.41
1:A:219:PRO:CB	1:A:290:LYS:HB3	2.31	0.41
1:A:50:ILE:HB	1:A:387:ARG:HG2	2.03	0.41
1:A:25:LYS:C	1:A:28:PRO:HD2	2.41	0.41
1:A:193:LYS:HG3	1:A:343:LYS:O	2.21	0.41
1:A:285:SER:H	1:A:362:PRO:CB	2.31	0.40
1:A:143:PHE:CD1	1:A:143:PHE:N	2.89	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:PRO:HB3	1:A:259:LYS:O	2.21	0.40
1:A:49:ASN:HD21	1:A:293:ILE:HG21	1.86	0.40
1:A:231:HIS:CE1	1:A:232:CYS:O	2.74	0.40
1:A:84:LEU:H	1:A:84:LEU:CD1	2.34	0.40
1:A:114:THR:CB	1:A:188:ILE:HA	2.52	0.40
1:A:283:SER:O	1:A:359:SER:HA	2.22	0.40
1:A:183:ALA:HB2	1:A:331:LYS:H	1.87	0.40
1:A:137:LEU:O	1:A:137:LEU:HD13	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	372/374 (100%)	228 (61%)	90 (24%)	54 (14%)	0 0

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	ILE
1	A	90	ALA
1	A	168	LYS
1	A	171	ASP
1	A	239	VAL
1	A	240	LEU
1	A	253	PHE
1	A	301	SER
1	A	310	LYS
1	A	311	VAL
1	A	330	SER
1	A	341	ASP
1	A	347	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	361	PRO
1	A	84	LEU
1	A	89	GLU
1	A	99	LEU
1	A	110	LEU
1	A	129	LYS
1	A	145	VAL
1	A	234	LYS
1	A	255	PRO
1	A	262	HIS
1	A	270	ASP
1	A	271	ILE
1	A	337	VAL
1	A	375	ILE
1	A	383	LEU
1	A	51	LEU
1	A	60	ALA
1	A	245	LEU
1	A	362	PRO
1	A	39	ARG
1	A	73	HIS
1	A	127	VAL
1	A	128	ASP
1	A	161	VAL
1	A	182	PHE
1	A	223	ARG
1	A	344	GLY
1	A	382	PRO
1	A	120	LEU
1	A	166	GLN
1	A	289	PRO
1	A	352	PHE
1	A	373	LEU
1	A	236	SER
1	A	336	ALA
1	A	360	ILE
1	A	307	GLY
1	A	167	GLY
1	A	173	VAL
1	A	210	VAL
1	A	308	ILE

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	328/328 (100%)	254 (77%)	74 (23%)	1 3

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ILE
1	A	29	ASN
1	A	38	TYR
1	A	40	GLN
1	A	43	HIS
1	A	49	ASN
1	A	56	SER
1	A	57	ILE
1	A	61	PHE
1	A	64	LEU
1	A	80	LEU
1	A	84	LEU
1	A	87	ILE
1	A	94	GLU
1	A	97	GLN
1	A	100	LEU
1	A	101	ARG
1	A	107	ASP
1	A	109	GLN
1	A	110	LEU
1	A	113	THR
1	A	120	LEU
1	A	122	GLU
1	A	125	LYS
1	A	130	PHE
1	A	133	ASP
1	A	138	TYR
1	A	139	HIS
1	A	150	THR
1	A	156	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	160	TYR
1	A	165	THR
1	A	171	ASP
1	A	176	LEU
1	A	177	ASP
1	A	179	ASP
1	A	189	PHE
1	A	191	LYS
1	A	194	TRP
1	A	199	GLU
1	A	203	THR
1	A	205	GLU
1	A	214	THR
1	A	215	THR
1	A	221	MET
1	A	229	ILE
1	A	235	LEU
1	A	249	THR
1	A	253	PHE
1	A	256	ASP
1	A	260	LEU
1	A	264	GLU
1	A	275	PHE
1	A	282	ARG
1	A	283	SER
1	A	285	SER
1	A	289	PRO
1	A	291	LEU
1	A	293	ILE
1	A	299	LEU
1	A	305	GLN
1	A	310	LYS
1	A	314	ASN
1	A	317	ASP
1	A	318	LEU
1	A	329	LEU
1	A	337	VAL
1	A	342	GLU
1	A	346	GLU
1	A	351	MET
1	A	373	LEU
1	A	383	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	385	MET
1	A	393	GLN

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

Mol	Chain	Res	Type
1	A	29	ASN
1	A	49	ASN
1	A	83	ASN
1	A	109	GLN
1	A	116	ASN
1	A	139	HIS
1	A	146	ASN
1	A	186	ASN
1	A	231	HIS
1	A	261	GLN
1	A	262	HIS
1	A	314	ASN
1	A	334	HIS
1	A	377	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 [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 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.