



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2017 – 12:31 AM EDT

PDB ID : 1CM7  
Title : 3-ISOPROPYLMALATE DEHYDROGENASE FROM ESCHERICHIA COLI  
Authors : Wallon, G.; Kryger, G.; Lovett, S.T.; Oshima, T.; Ringe, D.; Petsko, G.A.  
Deposited on : unknown  
Resolution : 2.06 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

<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  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

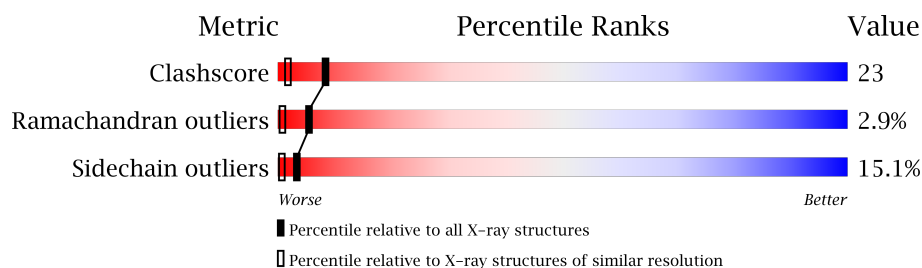
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.06 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	112137	2143 (2.08-2.04)
Ramachandran outliers	110173	2126 (2.08-2.04)
Sidechain outliers	110143	2126 (2.08-2.04)

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  $\geq 3$ , 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	363	
1	B	363	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5753 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 PROTEIN (3-ISOPROPYLMALATE DEHYDROGENASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	363	Total	C	N	O	S	0	0	0
			2763	1740	481	527	15			
1	B	363	Total	C	N	O	S	0	0	0
			2759	1738	481	526	14			

- Molecule 2 is water.

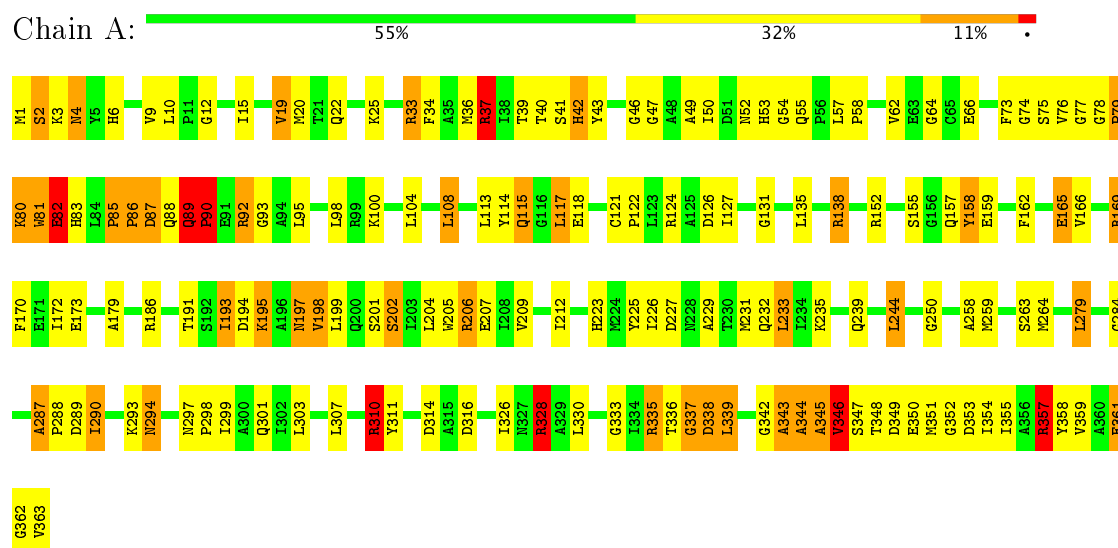
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	102	Total	O	0	0
			102	102		
2	B	129	Total	O	0	0
			129	129		

### 3 Residue-property plots

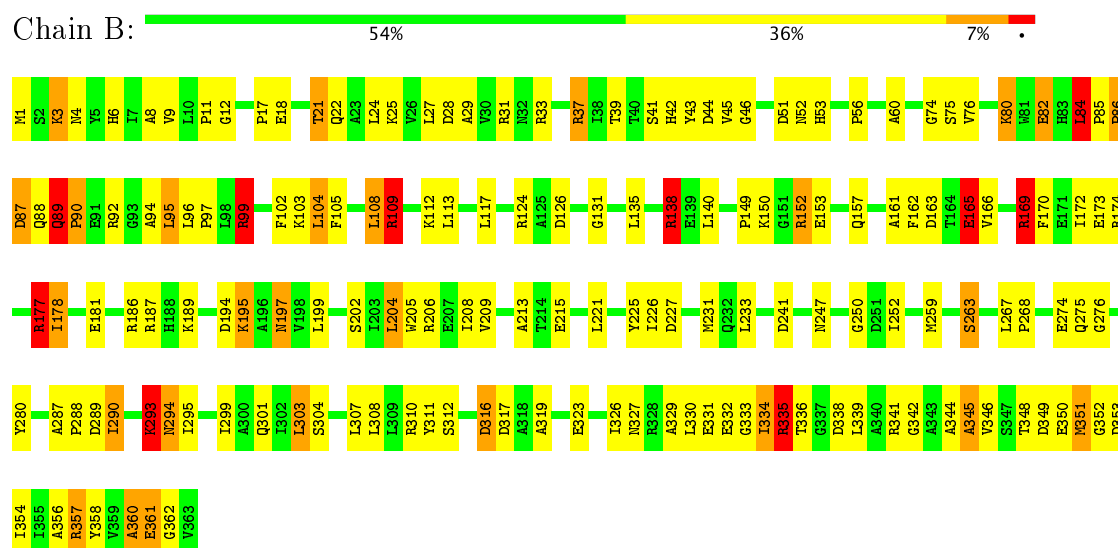
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: PROTEIN (3-ISOPROPYLMALATE DEHYDROGENASE)



#### • Molecule 1: PROTEIN (3-ISOPROPYLMALATE DEHYDROGENASE)



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.80 Å 86.90 Å 83.70 Å 90.00° 93.30° 90.00°	Depositor
Resolution (Å)	6.00 – 2.06	Depositor
% Data completeness (in resolution range)	79.0 (6.00-2.06)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.173 , 0.245	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5753	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	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	0.61	1/2816 (0.0%)	0.78	7/3814 (0.2%)
1	B	0.72	3/2813 (0.1%)	0.87	13/3813 (0.3%)
All	All	0.67	4/5629 (0.1%)	0.83	20/7627 (0.3%)

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
1	A	0	12
1	B	0	18
All	All	0	30

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	345	ALA	C-N	-21.37	0.84	1.34
1	A	81	TRP	C-N	-9.82	1.11	1.34
1	B	80	LYS	C-N	-7.62	1.16	1.34
1	B	335	ARG	C-N	5.65	1.47	1.34

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	345	ALA	C-N-CA	13.47	155.37	121.70
1	B	80	LYS	O-C-N	-11.63	104.08	122.70
1	A	310	ARG	NE-CZ-NH1	-9.68	115.46	120.30
1	B	335	ARG	O-C-N	-8.66	108.85	122.70
1	B	345	ALA	O-C-N	-8.11	109.72	122.70
1	B	293	LYS	N-CA-C	7.21	130.48	111.00
1	B	80	LYS	CA-C-N	6.98	132.55	117.20
1	A	346	VAL	C-N-CA	6.88	138.89	121.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	294	ASN	N-CA-C	6.56	128.71	111.00
1	B	335	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	B	169	ARG	NE-CZ-NH1	-6.05	117.28	120.30
1	A	357	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	B	345	ALA	CA-C-N	5.59	129.50	117.20
1	A	328	ARG	NE-CZ-NH1	-5.47	117.56	120.30
1	A	346	VAL	O-C-N	-5.40	114.06	122.70
1	B	204	LEU	CA-CB-CG	5.39	127.69	115.30
1	B	169	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	A	89	GLN	O-C-N	-5.19	111.23	121.10
1	A	10	LEU	CA-CB-CG	5.14	127.13	115.30
1	B	177	ARG	NE-CZ-NH2	-5.09	117.75	120.30

There are no chirality outliers.

All (30) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	158	TYR	Sidechain
1	A	169	ARG	Sidechain
1	A	186	ARG	Sidechain
1	A	287	ALA	Peptide
1	A	310	ARG	Sidechain
1	A	311	TYR	Sidechain
1	A	328	ARG	Sidechain
1	A	357	ARG	Sidechain
1	A	37	ARG	Sidechain
1	A	85	PRO	Peptide
1	A	87	ASP	Peptide
1	A	89	GLN	Peptide
1	B	1	MET	Peptide
1	B	109	ARG	Sidechain
1	B	138	ARG	Sidechain
1	B	165	GLU	Mainchain
1	B	169	ARG	Sidechain
1	B	177	ARG	Sidechain
1	B	186	ARG	Sidechain
1	B	206	ARG	Sidechain
1	B	31	ARG	Sidechain
1	B	311	TYR	Sidechain
1	B	335	ARG	Sidechain,Mainchain
1	B	360	ALA	Peptide
1	B	43	TYR	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
1	B	80	LYS	Mainchain
1	B	84	LEU	Peptide
1	B	89	GLN	Peptide
1	B	99	ARG	Sidechain

## 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	2763	0	2720	136	37
1	B	2759	0	2711	126	73
2	A	102	0	0	5	5
2	B	129	0	0	12	10
All	All	5753	0	5431	254	77

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 23.

All (254) 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:B:345:ALA:O	1:B:346:VAL:N	1.72	1.19
1:B:88:GLN:C	1:B:89:GLN:HG2	1.55	1.18
1:B:345:ALA:CA	1:B:346:VAL:N	2.13	1.11
1:A:338:ASP:C	1:A:339:LEU:N	2.05	1.10
1:B:88:GLN:O	1:B:89:GLN:HG2	1.52	1.07
1:A:338:ASP:O	1:A:339:LEU:N	1.88	1.06
1:A:346:VAL:HG22	1:A:350:GLU:HB3	1.34	1.06
1:B:345:ALA:C	1:B:346:VAL:CA	2.27	1.03
1:B:22:GLN:HE21	1:B:352:GLY:HA3	1.30	0.95
1:B:345:ALA:C	1:B:346:VAL:N	0.84	0.89
1:B:88:GLN:O	1:B:89:GLN:CG	2.20	0.89
1:B:357:ARG:HH11	1:B:357:ARG:HG3	1.38	0.88
1:B:335:ARG:HD3	1:B:338:ASP:HB2	1.56	0.86
1:A:52:ASN:HB3	1:A:53:HIS:CE1	2.15	0.81
1:B:18:GLU:HG2	1:B:293:LYS:HD2	1.62	0.81

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:ASN:HD22	1:A:348:THR:HB	1.46	0.79
1:A:358:TYR:CE1	1:A:363:VAL:HB	2.17	0.79
1:A:199:LEU:HB2	1:A:202:SER:HB2	1.67	0.77
1:A:62:VAL:O	1:A:66:GLU:HG3	1.83	0.77
1:A:287:ALA:HB3	1:A:288:PRO:HA	1.66	0.77
1:B:195:LYS:HB3	1:B:199:LEU:HD12	1.66	0.76
1:A:33:ARG:HD2	1:A:34:PHE:CE2	2.21	0.75
1:A:89:GLN:CB	1:A:92:ARG:HE	2.01	0.74
1:A:335:ARG:HD3	1:A:339:LEU:HB2	1.70	0.72
1:A:299:ILE:HG12	1:A:326:ILE:HD12	1.71	0.72
1:B:108:LEU:HD21	1:B:178:ILE:HD11	1.71	0.71
1:A:294:ASN:ND2	1:A:348:THR:HB	2.05	0.71
1:A:86:PRO:O	1:A:92:ARG:HB2	1.91	0.71
1:A:328:ARG:NH1	1:A:363:VAL:HG12	2.05	0.70
1:B:6:HIS:HE1	2:B:369:HOH:O	1.74	0.70
1:B:12:GLY:HA3	1:B:75:SER:O	1.92	0.69
1:A:346:VAL:CG2	1:A:350:GLU:HB3	2.16	0.69
1:B:333:GLY:HA2	1:B:335:ARG:NH2	2.08	0.69
1:A:46:GLY:O	1:A:50:ILE:HG12	1.93	0.69
1:B:263:SER:HB2	2:B:396:HOH:O	1.92	0.68
1:B:333:GLY:HA2	1:B:335:ARG:HH22	1.59	0.68
1:B:84:LEU:HB3	1:B:85:PRO:HD3	1.76	0.67
1:A:3:LYS:O	1:A:4:ASN:HB2	1.94	0.67
1:A:335:ARG:HD3	1:A:339:LEU:CB	2.24	0.67
1:A:335:ARG:HD3	1:A:338:ASP:O	1.95	0.66
1:B:88:GLN:C	1:B:89:GLN:CG	2.43	0.66
1:A:197:ASN:H	1:A:197:ASN:ND2	1.93	0.66
1:A:358:TYR:HE1	1:A:363:VAL:HB	1.57	0.65
1:B:41:SER:HB2	2:B:483:HOH:O	1.96	0.65
1:A:197:ASN:HD22	1:A:197:ASN:N	1.94	0.65
1:B:150:LYS:HE2	1:B:163:ASP:OD1	1.95	0.65
1:B:22:GLN:HE22	1:B:25:LYS:NZ	1.94	0.65
1:A:19:VAL:HG22	1:A:298:PRO:HA	1.78	0.65
1:A:80:LYS:O	1:A:80:LYS:HG2	1.96	0.65
1:A:22:GLN:HE21	1:A:352:GLY:HA3	1.61	0.65
1:B:8:ALA:HA	2:B:483:HOH:O	1.97	0.65
1:B:268:PRO:HG3	1:B:303:LEU:HB3	1.78	0.64
1:B:124:ARG:HD2	1:B:126:ASP:OD1	1.97	0.64
1:B:56:PRO:HG3	1:B:89:GLN:HA	1.78	0.64
1:A:194:ASP:O	1:A:225:TYR:HA	1.98	0.63
1:B:290:ILE:HG13	1:B:295:ILE:HD11	1.80	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:GLY:HA2	1:B:301:GLN:HE22	1.63	0.63
1:A:155:SER:HA	1:A:159:GLU:HB2	1.81	0.63
1:A:12:GLY:HA3	1:A:75:SER:O	1.99	0.63
1:A:2:SER:H	1:A:36:MET:HG2	1.63	0.63
1:A:346:VAL:HG22	1:A:350:GLU:CB	2.19	0.62
1:A:92:ARG:NE	1:A:92:ARG:H	1.97	0.62
1:B:197:ASN:N	1:B:197:ASN:HD22	1.96	0.62
1:B:46:GLY:HA3	1:B:76:VAL:CG2	2.29	0.62
1:A:22:GLN:HE22	1:A:25:LYS:NZ	1.97	0.62
1:A:346:VAL:HG21	1:A:354:ILE:HD12	1.81	0.62
1:B:138:ARG:NH1	1:B:247:ASN:OD1	2.31	0.62
1:A:316:ASP:HB2	2:A:434:HOH:O	1.99	0.62
1:B:17:PRO:O	1:B:21:THR:HG23	2.00	0.62
1:B:109:ARG:HB3	1:B:109:ARG:CZ	2.30	0.61
1:A:357:ARG:HH21	1:A:363:VAL:HG21	1.65	0.61
1:B:294:ASN:ND2	1:B:348:THR:HB	2.14	0.61
1:B:87:ASP:HA	1:B:92:ARG:HB3	1.81	0.61
1:A:46:GLY:HA3	1:A:76:VAL:CG2	2.29	0.61
1:A:47:GLY:O	1:A:50:ILE:HB	2.00	0.61
1:A:350:GLU:O	1:A:354:ILE:HG13	2.02	0.60
1:A:351:MET:O	1:A:355:ILE:HG12	2.02	0.59
1:A:287:ALA:CB	1:A:288:PRO:HA	2.32	0.59
1:A:15:ILE:HG23	1:A:287:ALA:CB	2.33	0.58
1:A:1:MET:HG3	1:A:34:PHE:O	2.04	0.58
1:A:9:VAL:HG13	1:A:20:MET:HE3	1.86	0.58
1:A:22:GLN:HE22	1:A:25:LYS:HZ1	1.51	0.57
1:B:323:GLU:HB3	2:B:487:HOH:O	2.03	0.57
1:B:109:ARG:HH22	1:B:267:LEU:HD13	1.70	0.57
1:A:328:ARG:HH12	1:A:363:VAL:HG12	1.68	0.57
1:A:15:ILE:HG23	1:A:287:ALA:HB2	1.87	0.57
1:B:113:LEU:HD23	1:B:131:GLY:HA2	1.86	0.57
1:B:336:THR:HG23	1:B:351:MET:HG3	1.87	0.57
1:A:335:ARG:HG2	1:A:338:ASP:HB2	1.87	0.56
1:A:92:ARG:H	1:A:92:ARG:HE	1.53	0.56
1:B:194:ASP:O	1:B:225:TYR:HA	2.04	0.56
1:B:108:LEU:CD2	1:B:178:ILE:HD11	2.35	0.56
1:A:349:ASP:HB3	2:A:415:HOH:O	2.05	0.56
1:B:18:GLU:HG2	1:B:293:LYS:HA	1.88	0.56
1:A:49:ALA:HB1	1:A:58:PRO:CG	2.36	0.55
1:B:149:PRO:HB2	1:B:162:PHE:HE2	1.72	0.55
1:B:187:ARG:HD3	2:B:476:HOH:O	2.06	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:ILE:O	1:A:54:GLY:HA2	2.07	0.55
1:B:299:ILE:HG23	1:B:326:ILE:HD12	1.88	0.55
1:A:43:TYR:CZ	1:A:64:GLY:HA3	2.42	0.55
1:B:197:ASN:N	1:B:197:ASN:ND2	2.53	0.55
1:B:327:ASN:O	1:B:331:GLU:HG2	2.07	0.55
1:B:350:GLU:O	1:B:354:ILE:HG13	2.07	0.54
1:A:52:ASN:HB3	1:A:53:HIS:ND1	2.22	0.54
1:A:197:ASN:HD22	1:A:197:ASN:H	1.52	0.54
1:A:205:TRP:O	1:A:209:VAL:HG23	2.08	0.54
1:B:172:ILE:HD13	1:B:205:TRP:HA	1.89	0.54
1:B:310:ARG:HD3	1:B:316:ASP:HB3	1.90	0.54
1:A:138:ARG:HG3	1:A:250:GLY:HA3	1.89	0.54
1:A:108:LEU:HB3	1:A:135:LEU:HD11	1.90	0.53
1:A:335:ARG:CD	1:A:339:LEU:CB	2.87	0.53
1:A:89:GLN:CB	1:A:92:ARG:NE	2.71	0.53
1:A:170:PHE:HB3	1:B:157:GLN:HG2	1.91	0.53
1:A:344:ALA:O	1:A:346:VAL:N	2.41	0.53
1:B:195:LYS:HD3	1:B:226:ILE:HG22	1.89	0.53
1:B:194:ASP:HB2	1:B:202:SER:HB3	1.89	0.53
1:A:114:TYR:O	1:A:117:LEU:HD22	2.09	0.52
1:A:195:LYS:HE2	1:A:197:ASN:HD21	1.74	0.52
1:A:172:ILE:HD13	1:A:205:TRP:HA	1.90	0.52
1:A:42:HIS:CD2	1:A:42:HIS:C	2.83	0.52
1:B:197:ASN:ND2	1:B:197:ASN:H	2.06	0.52
1:A:46:GLY:HA3	1:A:76:VAL:HG23	1.91	0.52
1:B:299:ILE:HG12	1:B:326:ILE:HD13	1.92	0.52
1:B:3:LYS:CB	1:B:37:ARG:H	2.22	0.52
1:A:259:MET:HB2	1:B:231:MET:HE2	1.92	0.52
1:A:342:GLY:O	1:A:343:ALA:HB3	2.10	0.51
1:A:89:GLN:O	1:A:93:GLY:HA3	2.09	0.51
1:B:11:PRO:HD2	2:B:388:HOH:O	2.09	0.51
1:B:360:ALA:O	1:B:361:GLU:HB2	2.09	0.51
1:B:95:LEU:O	1:B:99:ARG:HG2	2.09	0.51
1:A:81:TRP:O	1:A:82:GLU:C	2.47	0.51
1:B:346:VAL:HG13	1:B:350:GLU:HB3	1.92	0.51
1:A:74:GLY:HA2	1:A:301:GLN:HE22	1.75	0.51
1:A:20:MET:HB2	2:A:439:HOH:O	2.11	0.50
1:B:294:ASN:HD22	1:B:348:THR:HB	1.75	0.50
1:B:99:ARG:HD2	1:B:104:LEU:HD23	1.93	0.50
1:B:357:ARG:HG3	2:B:455:HOH:O	2.11	0.49
1:A:232:GLN:NE2	1:A:239:GLN:HE22	2.10	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:VAL:C	1:A:361:GLU:H	2.16	0.49
1:B:357:ARG:HH11	1:B:357:ARG:CG	2.19	0.49
1:A:229:ALA:O	1:A:233:LEU:HD22	2.13	0.49
1:A:297:ASN:HA	1:A:336:THR:HG21	1.94	0.49
1:A:6:HIS:CE1	1:A:41:SER:HG	2.30	0.49
1:B:108:LEU:HD21	1:B:178:ILE:CD1	2.42	0.48
1:A:42:HIS:CD2	1:A:43:TYR:N	2.82	0.48
1:B:310:ARG:NH1	1:B:319:ALA:HB3	2.28	0.48
1:A:335:ARG:HB3	1:A:337:GLY:H	1.78	0.48
1:A:50:ILE:HG21	1:A:81:TRP:CD1	2.48	0.48
1:B:150:LYS:HG2	2:B:377:HOH:O	2.14	0.48
1:A:162:PHE:HA	1:B:165:GLU:O	2.13	0.48
1:B:205:TRP:O	1:B:209:VAL:HG23	2.13	0.48
1:A:152:ARG:HD2	2:B:382:HOH:O	2.13	0.48
1:B:46:GLY:HA3	1:B:76:VAL:HG21	1.94	0.48
1:A:165:GLU:O	1:B:162:PHE:HA	2.14	0.48
1:A:346:VAL:HG13	1:A:347:SER:O	2.14	0.48
1:A:358:TYR:CD1	1:A:363:VAL:HB	2.49	0.48
1:B:357:ARG:NH1	1:B:357:ARG:HG3	2.17	0.48
1:B:6:HIS:HD2	1:B:39:THR:CG2	2.27	0.48
1:A:197:ASN:N	1:A:197:ASN:ND2	2.52	0.47
1:A:53:HIS:O	1:A:55:GLN:HG3	2.15	0.47
1:B:138:ARG:CG	1:B:250:GLY:HA3	2.45	0.47
1:B:44:ASP:OD2	1:B:53:HIS:HE1	1.98	0.47
1:B:88:GLN:O	1:B:89:GLN:CD	2.53	0.47
1:B:173:GLU:O	1:B:177:ARG:HG2	2.15	0.46
1:A:357:ARG:NH2	1:A:363:VAL:HG21	2.30	0.46
1:A:50:ILE:HG21	1:A:81:TRP:HD1	1.80	0.46
1:A:191:THR:HG22	1:A:193:ILE:CD1	2.46	0.46
1:A:310:ARG:HE	1:A:310:ARG:HB2	1.32	0.46
1:A:86:PRO:O	1:A:92:ARG:CB	2.63	0.46
1:B:102:PHE:O	1:B:103:LYS:HB2	2.15	0.46
1:B:358:TYR:O	1:B:361:GLU:HA	2.15	0.46
1:A:76:VAL:HG22	1:A:90:PRO:HB3	1.97	0.46
1:B:84:LEU:HD22	1:B:85:PRO:HG3	1.98	0.46
1:B:335:ARG:HA	1:B:351:MET:HE2	1.97	0.46
1:A:76:VAL:HG13	1:A:76:VAL:O	2.16	0.46
1:B:301:GLN:O	1:B:304:SER:HB2	2.16	0.46
1:B:96:LEU:H	1:B:97:PRO:HD2	1.80	0.46
1:A:346:VAL:HG21	1:A:354:ILE:CD1	2.46	0.46
1:A:77:GLY:O	1:A:81:TRP:CE3	2.69	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:VAL:HG13	1:A:301:GLN:HB2	1.98	0.45
1:B:152:ARG:HG3	1:B:153:GLU:N	2.31	0.45
1:A:179:ALA:CB	1:A:244:LEU:HG	2.46	0.45
1:A:15:ILE:H	1:A:287:ALA:HB2	1.80	0.45
1:A:206:ARG:HD2	1:A:223:HIS:ND1	2.32	0.45
1:B:84:LEU:CB	1:B:85:PRO:HD3	2.45	0.45
1:A:232:GLN:OE1	1:A:235:LYS:HD2	2.16	0.45
1:B:6:HIS:HD2	1:B:39:THR:HB	1.81	0.45
1:B:84:LEU:HB3	1:B:85:PRO:CD	2.45	0.45
1:A:201:SER:HA	1:B:161:ALA:HB3	1.99	0.45
1:A:353:ASP:O	1:A:357:ARG:HB2	2.17	0.44
1:B:117:LEU:HD21	1:B:335:ARG:HH11	1.81	0.44
1:B:105:PHE:CE1	1:B:174:ARG:HG3	2.52	0.44
1:B:189:LYS:HB2	1:B:241:ASP:HB3	2.00	0.44
1:B:329:ALA:O	1:B:332:GLU:HB2	2.18	0.44
1:A:121:CYS:HA	1:A:122:PRO:HD3	1.80	0.44
1:A:73:PHE:CD1	1:A:74:GLY:N	2.86	0.44
1:A:333:GLY:HA2	1:A:335:ARG:HH21	1.83	0.44
1:A:335:ARG:HG2	1:A:338:ASP:CB	2.47	0.44
1:B:108:LEU:HD23	1:B:108:LEU:N	2.33	0.44
1:A:195:LYS:HD3	1:A:226:ILE:HG22	2.00	0.44
1:A:335:ARG:HD3	1:A:339:LEU:N	2.32	0.44
1:B:335:ARG:HD2	1:B:339:LEU:HB2	1.99	0.44
1:A:108:LEU:N	1:A:108:LEU:HD23	2.32	0.43
1:A:290:ILE:HA	1:A:290:ILE:HD12	1.76	0.43
1:B:213:ALA:HB2	1:B:221:LEU:HD22	2.00	0.43
1:B:22:GLN:HE22	1:B:25:LYS:CE	2.29	0.43
1:A:301:GLN:NE2	2:A:439:HOH:O	2.50	0.43
1:B:195:LYS:O	1:B:197:ASN:ND2	2.51	0.43
1:B:287:ALA:HA	1:B:288:PRO:HD2	1.79	0.43
1:A:335:ARG:O	1:A:346:VAL:HG12	2.19	0.43
1:B:226:ILE:O	1:B:226:ILE:HD12	2.19	0.43
1:A:195:LYS:HA	1:A:195:LYS:HD2	1.68	0.43
1:A:80:LYS:HD3	1:A:80:LYS:H	1.83	0.43
1:B:169:ARG:HE	1:B:208:ILE:HD12	1.83	0.43
1:B:138:ARG:HG2	1:B:250:GLY:HA3	2.00	0.42
1:B:334:ILE:HG12	1:B:335:ARG:N	2.32	0.42
1:B:85:PRO:HD2	1:B:89:GLN:HG3	2.01	0.42
1:A:124:ARG:O	1:A:127:ILE:N	2.49	0.42
1:A:79:PRO:HG2	1:A:81:TRP:HH2	1.85	0.42
1:B:299:ILE:HG12	1:B:326:ILE:CD1	2.49	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:VAL:HG22	1:B:46:GLY:N	2.35	0.42
1:B:105:PHE:HE2	1:B:274:GLU:HG2	1.84	0.42
1:A:289:ASP:OD2	1:A:290:ILE:HD13	2.20	0.42
1:B:334:ILE:HA	2:B:442:HOH:O	2.20	0.42
1:B:90:PRO:O	1:B:94:ALA:HB3	2.20	0.42
1:B:17:PRO:O	1:B:21:THR:CG2	2.68	0.42
1:B:199:LEU:HB2	1:B:202:SER:HB2	2.02	0.42
1:B:18:GLU:CD	1:B:293:LYS:HA	2.40	0.42
1:A:113:LEU:HD23	1:A:131:GLY:HA2	2.02	0.41
1:B:86:PRO:O	1:B:92:ARG:HB2	2.20	0.41
1:B:9:VAL:O	1:B:42:HIS:HA	2.19	0.41
1:A:263:SER:O	1:A:264:MET:HB2	2.20	0.41
1:A:6:HIS:HA	1:A:39:THR:O	2.20	0.41
1:A:115:GLN:HG2	1:A:118:GLU:OE2	2.20	0.41
1:A:227:ASP:HB3	1:B:252:ILE:HA	2.03	0.41
1:A:231:MET:HB3	1:B:259:MET:CE	2.51	0.41
1:A:258:ALA:O	1:A:264:MET:HG2	2.20	0.41
1:A:284:GLY:HA3	2:A:458:HOH:O	2.20	0.41
1:A:79:PRO:HG2	1:A:81:TRP:CH2	2.56	0.41
1:B:99:ARG:HH22	1:B:140:LEU:HD13	1.86	0.41
1:B:18:GLU:CG	1:B:293:LYS:HA	2.50	0.41
1:B:29:ALA:HA	2:B:471:HOH:O	2.20	0.41
1:A:169:ARG:HD3	1:A:173:GLU:OE2	2.20	0.41
1:A:343:ALA:O	1:A:345:ALA:N	2.54	0.41
1:B:329:ALA:O	1:B:334:ILE:HG23	2.21	0.41
1:A:15:ILE:N	1:A:287:ALA:HB2	2.36	0.41
1:A:19:VAL:HG13	1:A:301:GLN:CB	2.51	0.41
1:B:6:HIS:HD2	1:B:39:THR:HG22	1.85	0.41
1:B:361:GLU:OE1	1:B:361:GLU:HA	2.21	0.40
1:A:124:ARG:HD2	1:A:126:ASP:OD1	2.22	0.40
1:B:99:ARG:HA	1:B:104:LEU:HD22	2.03	0.40
1:A:198:VAL:O	1:B:150:LYS:NZ	2.52	0.40
1:A:95:LEU:HD11	1:A:279:LEU:HD21	2.04	0.40
1:B:280:TYR:CZ	1:B:308:LEU:HA	2.57	0.40

All (77) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:GLN:CD	1:B:353:ASP:O[2_647]	0.97	1.23

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:GLN:OE1	2:B:455:HOH:O[2_647]	0.99	1.21
1:A:158:TYR:OH	1:B:362:GLY:O[2_647]	1.05	1.15
1:B:276:GLY:CA	1:B:342:GLY:O[2_647]	1.13	1.07
1:A:39:THR:CA	1:B:52:ASN:O[1_554]	1.15	1.05
1:B:215:GLU:OE1	2:B:441:HOH:O[2_647]	1.22	0.98
1:A:40:THR:O	1:B:53:HIS:CD2[1_554]	1.23	0.97
1:A:37:ARG:NH2	1:B:51:ASP:O[1_554]	1.31	0.89
1:B:356:ALA:O	2:A:420:HOH:O[2_657]	1.31	0.89
1:B:170:PHE:CG	1:B:357:ARG:NH1[2_647]	1.34	0.86
1:A:157:GLN:CG	1:B:353:ASP:O[2_647]	1.40	0.80
1:B:349:ASP:OD1	2:B:454:HOH:O[2_657]	1.41	0.79
1:B:170:PHE:CB	1:B:357:ARG:NH1[2_647]	1.43	0.77
1:A:157:GLN:NE2	1:B:353:ASP:CA[2_647]	1.46	0.74
1:B:360:ALA:CB	2:A:426:HOH:O[2_657]	1.50	0.70
1:B:173:GLU:OE2	1:B:353:ASP:CG[2_647]	1.50	0.70
1:B:177:ARG:NH2	1:B:350:GLU:N[2_647]	1.52	0.68
1:A:158:TYR:OH	1:B:362:GLY:C[2_647]	1.54	0.66
1:A:362:GLY:O	2:B:482:HOH:O[2_756]	1.58	0.62
1:A:158:TYR:CZ	1:B:362:GLY:O[2_647]	1.59	0.61
1:B:215:GLU:OE2	1:B:349:ASP:CB[2_647]	1.59	0.61
1:A:157:GLN:NE2	1:B:353:ASP:C[2_647]	1.61	0.59
1:A:157:GLN:NE2	1:B:353:ASP:O[2_647]	1.63	0.57
1:B:177:ARG:NH1	1:B:350:GLU:CB[2_647]	1.64	0.56
1:B:173:GLU:OE2	1:B:353:ASP:OD2[2_647]	1.67	0.53
1:B:60:ALA:CB	2:A:383:HOH:O[1_556]	1.72	0.48
1:A:157:GLN:CD	1:B:353:ASP:C[2_647]	1.73	0.47
1:A:157:GLN:CB	1:B:357:ARG:CA[2_647]	1.74	0.46
1:A:37:ARG:NH2	1:B:51:ASP:C[1_554]	1.75	0.45
1:B:170:PHE:CG	1:B:357:ARG:CZ[2_647]	1.79	0.41
1:B:177:ARG:NH1	1:B:350:GLU:CG[2_647]	1.79	0.41
1:A:157:GLN:CB	1:B:357:ARG:CB[2_647]	1.80	0.40
1:A:158:TYR:CZ	1:B:362:GLY:C[2_647]	1.81	0.39
1:B:349:ASP:CG	2:B:454:HOH:O[2_657]	1.85	0.35
1:B:177:ARG:CZ	1:B:350:GLU:CB[2_647]	1.85	0.35
1:A:39:THR:C	1:B:52:ASN:O[1_554]	1.86	0.34
1:A:39:THR:CB	1:B:52:ASN:O[1_554]	1.86	0.34
1:A:157:GLN:OE1	1:B:353:ASP:O[2_647]	1.87	0.33
1:A:158:TYR:CE1	1:B:362:GLY:O[2_647]	1.88	0.32
1:B:356:ALA:C	2:A:420:HOH:O[2_657]	1.90	0.30
1:A:158:TYR:OH	1:B:362:GLY:CA[2_647]	1.91	0.29
1:A:157:GLN:CG	1:B:357:ARG:N[2_647]	1.92	0.28

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:GLU:CG	2:B:385:HOH:O[2_657]	1.92	0.28
1:B:173:GLU:OE2	1:B:353:ASP:CB[2_647]	1.93	0.27
1:B:177:ARG:CG	1:B:350:GLU:OE1[2_647]	1.97	0.23
1:B:170:PHE:CE1	1:B:357:ARG:NH2[2_647]	1.97	0.23
1:A:40:THR:O	1:B:53:HIS:CG[1_554]	1.98	0.22
1:B:177:ARG:NH2	1:B:350:GLU:CA[2_647]	1.98	0.22
1:A:37:ARG:NH2	1:B:51:ASP:CA[1_554]	1.98	0.22
1:B:170:PHE:CD2	1:B:357:ARG:CZ[2_647]	1.98	0.22
1:B:353:ASP:OD2	2:B:449:HOH:O[2_657]	1.99	0.21
1:B:215:GLU:OE2	1:B:349:ASP:CG[2_647]	1.99	0.21
1:B:170:PHE:CD1	1:B:357:ARG:NH1[2_647]	2.00	0.20
1:B:60:ALA:N	2:A:383:HOH:O[1_556]	2.01	0.19
1:A:157:GLN:CB	1:B:357:ARG:N[2_647]	2.04	0.16
1:B:215:GLU:CD	2:B:441:HOH:O[2_647]	2.05	0.15
1:A:40:THR:C	1:B:53:HIS:CD2[1_554]	2.05	0.15
1:A:157:GLN:CB	1:B:357:ARG:CG[2_647]	2.05	0.15
1:B:177:ARG:NH1	1:B:350:GLU:CA[2_647]	2.06	0.14
1:A:40:THR:N	1:B:52:ASN:O[1_554]	2.06	0.14
1:B:215:GLU:CG	1:B:349:ASP:OD2[2_647]	2.06	0.14
1:B:170:PHE:CD1	1:B:357:ARG:NH2[2_647]	2.06	0.14
1:B:312:SER:O	1:B:341:ARG:O[2_647]	2.08	0.12
1:A:155:SER:OG	2:B:418:HOH:O[2_647]	2.08	0.12
1:A:39:THR:CA	1:B:52:ASN:C[1_554]	2.09	0.11
1:A:40:THR:OG1	1:B:53:HIS:NE2[1_554]	2.09	0.11
1:A:158:TYR:CE2	1:B:362:GLY:N[2_647]	2.10	0.10
1:B:275:GLN:O	1:B:344:ALA:CB[2_647]	2.11	0.09
1:B:215:GLU:OE2	1:B:349:ASP:OD2[2_647]	2.14	0.06
1:A:157:GLN:NE2	1:B:353:ASP:CB[2_647]	2.14	0.06
1:A:39:THR:CB	1:B:52:ASN:C[1_554]	2.16	0.04
1:B:170:PHE:CD1	1:B:357:ARG:CZ[2_647]	2.16	0.04
1:A:157:GLN:CD	2:B:455:HOH:O[2_647]	2.16	0.04
1:B:177:ARG:NE	1:B:350:GLU:OE1[2_647]	2.18	0.02
1:B:177:ARG:CD	1:B:350:GLU:OE1[2_647]	2.19	0.01
1:B:276:GLY:C	1:B:342:GLY:O[2_647]	2.19	0.01
1:B:276:GLY:CA	1:B:342:GLY:C[2_647]	2.19	0.01



## 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	359/363 (99%)	311 (87%)	34 (10%)	14 (4%)	3	0
1	B	361/363 (99%)	323 (90%)	31 (9%)	7 (2%)	9	2
All	All	720/726 (99%)	634 (88%)	65 (9%)	21 (3%)	5	1

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	79	PRO
1	A	90	PRO
1	A	345	ALA
1	B	86	PRO
1	B	293	LYS
1	B	361	GLU
1	A	78	GLY
1	A	82	GLU
1	B	4	ASN
1	B	82	GLU
1	A	85	PRO
1	A	207	GLU
1	A	337	GLY
1	A	294	ASN
1	A	361	GLU
1	B	3	LYS
1	A	86	PRO
1	A	343	ALA
1	A	344	ALA
1	B	90	PRO

### 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	285/288 (99%)	239 (84%)	46 (16%)	3	0
1	B	283/288 (98%)	243 (86%)	40 (14%)	4	1
All	All	568/576 (99%)	482 (85%)	86 (15%)	3	1

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	19	VAL
1	A	33	ARG
1	A	37	ARG
1	A	42	HIS
1	A	57	LEU
1	A	80	LYS
1	A	82	GLU
1	A	83	HIS
1	A	87	ASP
1	A	88	GLN
1	A	90	PRO
1	A	92	ARG
1	A	98	LEU
1	A	100	LYS
1	A	104	LEU
1	A	108	LEU
1	A	115	GLN
1	A	117	LEU
1	A	138	ARG
1	A	165	GLU
1	A	166	VAL
1	A	193	ILE
1	A	195	LYS
1	A	197	ASN
1	A	198	VAL
1	A	202	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	204	LEU
1	A	206	ARG
1	A	212	ILE
1	A	233	LEU
1	A	244	LEU
1	A	279	LEU
1	A	290	ILE
1	A	293	LYS
1	A	303	LEU
1	A	307	LEU
1	A	310	ARG
1	A	314	ASP
1	A	328	ARG
1	A	330	LEU
1	A	335	ARG
1	A	338	ASP
1	A	339	LEU
1	A	346	VAL
1	A	357	ARG
1	B	21	THR
1	B	24	LEU
1	B	27	LEU
1	B	28	ASP
1	B	33	ARG
1	B	37	ARG
1	B	82	GLU
1	B	84	LEU
1	B	87	ASP
1	B	89	GLN
1	B	95	LEU
1	B	99	ARG
1	B	104	LEU
1	B	108	LEU
1	B	109	ARG
1	B	112	LYS
1	B	135	LEU
1	B	138	ARG
1	B	152	ARG
1	B	165	GLU
1	B	166	VAL
1	B	178	ILE
1	B	181	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	195	LYS
1	B	197	ASN
1	B	204	LEU
1	B	227	ASP
1	B	233	LEU
1	B	263	SER
1	B	289	ASP
1	B	290	ILE
1	B	303	LEU
1	B	307	LEU
1	B	316	ASP
1	B	317	ASP
1	B	330	LEU
1	B	334	ILE
1	B	335	ARG
1	B	351	MET
1	B	357	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	42	HIS
1	A	107	ASN
1	A	157	GLN
1	A	188	HIS
1	A	197	ASN
1	A	232	GLN
1	A	294	ASN
1	A	301	GLN
1	B	6	HIS
1	B	22	GLN
1	B	53	HIS
1	B	89	GLN
1	B	168	HIS
1	B	197	ASN
1	B	294	ASN
1	B	301	GLN

### 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	2
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	338:ASP	C	339:LEU	N	2.05
1	B	80:LYS	C	81:TRP	N	1.16
1	A	81:TRP	C	82:GLU	N	1.11
1	B	345:ALA	C	346:VAL	N	0.84

## 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.