



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:33 PM UTC

PDB ID : 2ALD / pdb_00002ald
Title : HUMAN MUSCLE ALDOLASE
Authors : Dalby, A.R.; Littlechild, J.A.
Deposited on : 1998-10-21
Resolution : 2.10 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Xtriage (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

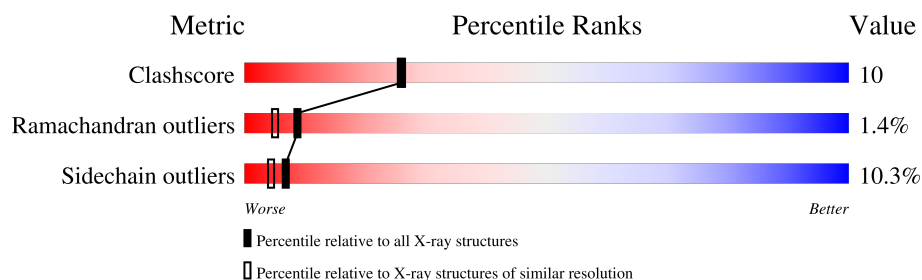
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

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 ≥ 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	363	 61% 30% 7% •

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2906 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 FRUCTOSE-BISPHOSPHATE ALDOLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	363	Total	C	N	O	S	45	0	0
			2763	1741	486	525	11			

- Molecule 2 is water.

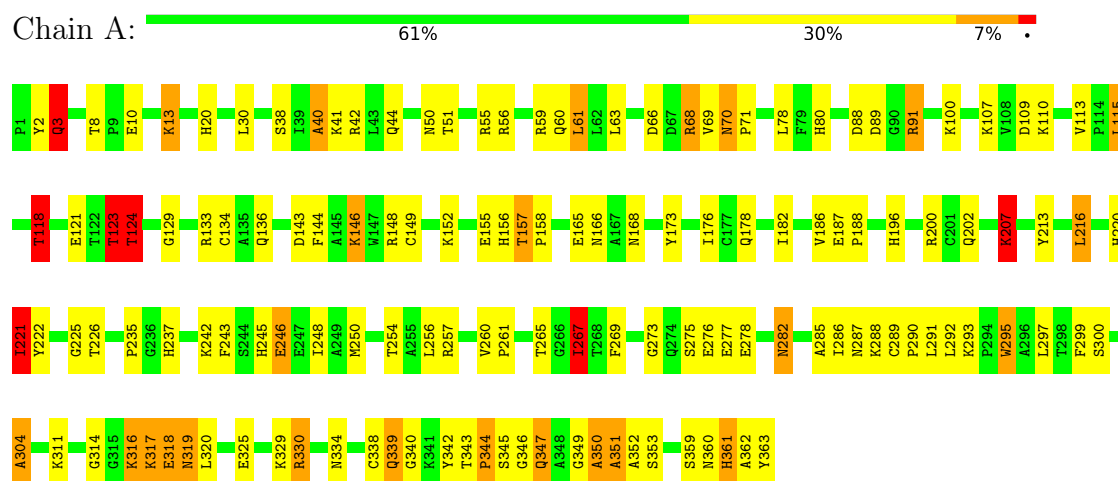
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	143	Total	O	0	0
			143	143		

3 Residue-property plots

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: FRUCTOSE-BISPHOSPHATE ALDOLASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, α , β , γ	96.50Å 96.50Å 167.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.10	Depositor
% Data completeness (in resolution range)	78.7 (20.00-2.10)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.172 , 0.258	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2906	wwPDB-VP
Average B, all atoms (Å ²)	31.0	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	1.20	3/2816 (0.1%)	2.18	111/3815 (2.9%)

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	16

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	350	ALA	C-N	27.26	1.71	1.33
1	A	344	PRO	C-N	19.83	1.61	1.33
1	A	330	ARG	CD-NE	-6.72	1.36	1.46

All (111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	330	ARG	CD-NE-CZ	32.43	169.81	124.40
1	A	343	THR	CA-C-O	-19.33	101.81	119.59
1	A	157	THR	CA-C-O	-14.06	106.17	120.66
1	A	343	THR	O-C-N	12.64	135.53	121.12
1	A	246	GLU	CB-CG-CD	11.74	132.55	112.60
1	A	352	ALA	CA-C-O	11.43	136.85	120.51
1	A	118	THR	N-CA-CB	-10.88	94.14	111.43
1	A	361	HIS	CA-CB-CG	9.83	123.63	113.80
1	A	133	ARG	NE-CZ-NH2	-9.73	110.45	119.20
1	A	168	ASN	OD1-CG-ND2	9.69	132.29	122.60
1	A	3	GLN	OE1-CD-NE2	9.45	132.04	122.60
1	A	344	PRO	O-C-N	-9.20	110.22	122.64
1	A	133	ARG	NE-CZ-NH1	8.74	130.24	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	123	THR	CB-CA-C	-8.49	94.86	112.44
1	A	243	PHE	CA-CB-CG	-8.45	105.35	113.80
1	A	157	THR	O-C-N	8.41	128.50	121.35
1	A	282	ASN	CA-CB-CG	-8.19	104.41	112.60
1	A	202	GLN	OE1-CD-NE2	-8.00	114.60	122.60
1	A	133	ARG	CD-NE-CZ	7.92	135.48	124.40
1	A	144	PHE	CA-CB-CG	7.69	121.49	113.80
1	A	221	ILE	CB-CG1-CD1	-7.65	97.74	113.80
1	A	267	ILE	CA-CB-CG2	7.58	123.39	110.50
1	A	202	GLN	CG-CD-NE2	7.38	127.46	116.40
1	A	237	HIS	CA-CB-CG	-7.36	106.44	113.80
1	A	213	TYR	CA-CB-CG	-7.32	100.73	113.90
1	A	123	THR	N-CA-CB	7.32	122.94	110.65
1	A	68	ARG	NE-CZ-NH2	-7.31	112.62	119.20
1	A	288	LYS	CA-C-O	-7.29	111.03	119.05
1	A	196	HIS	CA-CB-CG	-7.25	106.55	113.80
1	A	344	PRO	N-CA-CB	7.18	110.79	103.25
1	A	124	THR	CA-CB-OG1	7.17	120.36	109.60
1	A	350	ALA	O-C-N	-7.14	113.09	122.59
1	A	221	ILE	CB-CA-C	7.08	120.90	111.21
1	A	123	THR	OG1-CB-CG2	7.03	123.36	109.30
1	A	299	PHE	CA-C-O	-6.98	113.31	120.71
1	A	156	HIS	CA-CB-CG	-6.89	106.91	113.80
1	A	339	GLN	O-C-N	-6.75	114.05	122.35
1	A	143	ASP	CA-CB-CG	-6.73	105.87	112.60
1	A	243	PHE	CA-C-O	-6.72	113.51	121.11
1	A	235	PRO	CA-C-N	6.65	128.04	120.53
1	A	235	PRO	C-N-CA	6.65	128.04	120.53
1	A	110	LYS	CG-CD-CE	6.64	126.56	111.30
1	A	158	PRO	N-CA-CB	6.54	109.79	102.60
1	A	329	LYS	N-CA-CB	6.54	119.48	110.01
1	A	10	GLU	CB-CG-CD	6.46	123.58	112.60
1	A	221	ILE	CA-CB-CG2	6.41	121.39	110.50
1	A	124	THR	N-CA-CB	6.40	122.59	111.00
1	A	352	ALA	O-C-N	-6.38	114.11	122.59
1	A	288	LYS	O-C-N	6.37	130.18	122.35
1	A	109	ASP	CA-CB-CG	6.32	118.92	112.60
1	A	334	ASN	CA-CB-CG	-6.32	106.28	112.60
1	A	289	CYS	CA-C-O	6.19	124.98	119.59
1	A	2	TYR	N-CA-C	6.15	119.55	108.48
1	A	3	GLN	N-CA-C	6.12	119.49	109.76
1	A	40	ALA	CB-CA-C	-6.11	101.04	110.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	30	LEU	CA-C-N	-6.05	114.37	122.42
1	A	30	LEU	C-N-CA	-6.05	114.37	122.42
1	A	88	ASP	CA-CB-CG	-6.03	106.57	112.60
1	A	60	GLN	CB-CG-CD	-6.02	102.36	112.60
1	A	136	GLN	CA-C-O	6.02	126.90	120.70
1	A	146	LYS	CB-CG-CD	-5.97	97.57	111.30
1	A	311	LYS	CA-CB-CG	5.94	125.97	114.10
1	A	56	ARG	NE-CZ-NH1	5.93	127.43	121.50
1	A	118	THR	OG1-CB-CG2	5.89	121.08	109.30
1	A	344	PRO	N-CD-CG	5.89	112.03	103.20
1	A	113	VAL	N-CA-C	-5.87	104.38	109.19
1	A	343	THR	CB-CA-C	5.83	116.64	110.17
1	A	55	ARG	NE-CZ-NH1	5.82	127.32	121.50
1	A	257	ARG	CA-C-O	5.76	126.61	120.10
1	A	152	LYS	CA-C-O	-5.76	114.03	120.66
1	A	155	GLU	O-C-N	5.74	128.70	122.15
1	A	20	HIS	CA-CB-CG	-5.70	108.10	113.80
1	A	13	LYS	N-CA-C	-5.68	105.17	111.36
1	A	78	LEU	CA-C-N	5.61	129.44	121.42
1	A	78	LEU	C-N-CA	5.61	129.44	121.42
1	A	257	ARG	O-C-N	-5.58	115.69	122.22
1	A	330	ARG	NE-CZ-NH1	-5.58	115.92	121.50
1	A	260	VAL	CA-C-O	5.56	123.26	119.20
1	A	80	HIS	CA-CB-CG	-5.52	108.28	113.80
1	A	285	ALA	CA-C-O	5.51	126.33	120.10
1	A	248	ILE	CA-C-O	-5.48	115.25	120.95
1	A	166	ASN	CA-CB-CG	-5.48	107.12	112.60
1	A	293	LYS	CA-CB-CG	-5.44	103.22	114.10
1	A	220	HIS	CA-C-N	-5.43	113.81	122.50
1	A	220	HIS	C-N-CA	-5.43	113.81	122.50
1	A	176	ILE	CA-C-O	-5.39	115.35	120.95
1	A	109	ASP	CA-C-O	-5.35	115.49	121.81
1	A	123	THR	CA-CB-OG1	5.35	117.62	109.60
1	A	3	GLN	CB-CA-C	-5.34	101.13	109.84
1	A	286	ILE	N-CA-C	-5.28	105.35	110.42
1	A	349	GLY	N-CA-C	-5.27	106.02	112.77
1	A	340	GLY	N-CA-C	-5.26	105.74	114.48
1	A	353	SER	N-CA-C	-5.24	106.28	113.30
1	A	186	VAL	N-CA-CB	-5.24	105.03	111.00
1	A	42	ARG	CB-CA-C	5.24	119.75	110.85
1	A	295	TRP	CA-C-O	-5.20	115.53	121.40
1	A	282	ASN	CA-C-O	-5.19	114.92	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	68	ARG	CB-CG-CD	-5.17	99.41	111.30
1	A	319	ASN	CA-C-O	5.17	125.61	119.56
1	A	188	PRO	CA-C-O	-5.15	115.97	123.07
1	A	2	TYR	N-CA-CB	-5.13	102.20	110.71
1	A	207	LYS	CG-CD-CE	5.12	123.07	111.30
1	A	275	SER	N-CA-C	-5.11	103.94	110.53
1	A	256	LEU	O-C-N	-5.06	116.38	122.15
1	A	149	CYS	CA-C-O	-5.04	115.46	121.16
1	A	71	PRO	N-CA-CB	5.04	107.99	103.20
1	A	360	ASN	CA-CB-CG	5.04	117.64	112.60
1	A	304	ALA	CA-C-O	-5.04	110.85	118.91
1	A	265	THR	CA-C-O	5.01	125.73	120.42
1	A	330	ARG	CB-CG-CD	-5.00	99.79	111.30
1	A	61	LEU	CA-CB-CG	5.00	133.81	116.30

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	129	GLY	Mainchain
1	A	157	THR	Mainchain
1	A	225	GLY	Mainchain
1	A	254	THR	Mainchain
1	A	261	PRO	Mainchain
1	A	273	GLY	Mainchain
1	A	287	ASN	Mainchain
1	A	290	PRO	Mainchain
1	A	3	GLN	Mainchain
1	A	300	SER	Mainchain
1	A	314	GLY	Mainchain
1	A	338	CYS	Mainchain
1	A	339	GLN	Mainchain
1	A	344	PRO	Mainchain
1	A	51	THR	Mainchain
1	A	8	THR	Mainchain

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	2781	52	0
2	A	143	0	0	2	1
All	All	2906	0	2781	52	1

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 10.

All (52) 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:178:GLN:HE22	1:A:222:TYR:H	1.18	0.90
1:A:118:THR:HG23	1:A:121:GLU:H	1.37	0.87
1:A:66:ASP:OD1	1:A:68:ARG:HD3	1.76	0.85
1:A:89:ASP:OD1	1:A:91:ARG:HG2	1.82	0.78
1:A:118:THR:CG2	1:A:121:GLU:H	1.99	0.75
1:A:267:ILE:HG12	1:A:297:LEU:HD23	1.69	0.74
1:A:276:GLU:OE1	1:A:351:ALA:HB1	1.88	0.73
1:A:123:THR:HG21	1:A:165:GLU:OE2	1.88	0.72
1:A:330:ARG:HH11	1:A:351:ALA:HB3	1.55	0.71
1:A:123:THR:HG23	1:A:165:GLU:HG3	1.76	0.68
1:A:124:THR:HG21	1:A:148:ARG:O	1.94	0.67
1:A:70:ASN:HD21	1:A:100:LYS:HZ2	1.43	0.66
1:A:70:ASN:HD21	1:A:100:LYS:NZ	1.93	0.66
1:A:317:LYS:H	1:A:317:LYS:HE3	1.64	0.63
1:A:250:MET:HE1	1:A:291:LEU:HD11	1.80	0.63
1:A:361:HIS:CG	1:A:362:ALA:H	2.17	0.62
1:A:330:ARG:HE	1:A:351:ALA:HB3	1.67	0.59
1:A:221:ILE:HD11	1:A:226:THR:HG21	1.85	0.57
1:A:330:ARG:NH1	1:A:351:ALA:HB3	2.20	0.56
1:A:40:ALA:HB2	1:A:50:ASN:ND2	2.22	0.55
1:A:134:CYS:HB3	1:A:182:ILE:HD12	1.89	0.54
1:A:245:HIS:HD2	1:A:282:ASN:OD1	1.92	0.53
1:A:216:LEU:HG	1:A:221:ILE:HG12	1.92	0.52
1:A:267:ILE:HG12	1:A:297:LEU:CD2	2.40	0.52
1:A:250:MET:CE	1:A:291:LEU:HD11	2.39	0.52
1:A:40:ALA:HB2	1:A:50:ASN:HD22	1.75	0.51
1:A:178:GLN:HE22	1:A:222:TYR:N	1.99	0.50
1:A:68:ARG:NH1	1:A:325:GLU:OE2	2.42	0.50
1:A:267:ILE:HD11	1:A:269:PHE:CE1	2.46	0.50
1:A:317:LYS:HG2	1:A:318:GLU:OE2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:ARG:NE	1:A:351:ALA:HB3	2.26	0.49
1:A:267:ILE:HD11	1:A:269:PHE:CZ	2.49	0.47
1:A:115:LEU:O	1:A:118:THR:HB	2.15	0.47
1:A:267:ILE:O	1:A:267:ILE:HG13	2.10	0.46
1:A:207:LYS:HA	1:A:207:LYS:HD2	1.55	0.46
1:A:123:THR:HG22	1:A:124:THR:H	1.80	0.45
1:A:319:ASN:O	1:A:320:LEU:C	2.59	0.44
1:A:123:THR:CG2	1:A:165:GLU:HG3	2.43	0.44
1:A:245:HIS:CD2	1:A:282:ASN:OD1	2.71	0.44
1:A:148:ARG:HD3	2:A:456:HOH:O	2.18	0.44
1:A:200:ARG:HH11	1:A:200:ARG:HG3	1.83	0.44
1:A:178:GLN:NE2	1:A:222:TYR:H	1.99	0.43
1:A:276:GLU:HG2	1:A:304:ALA:O	2.18	0.43
1:A:316:LYS:HB3	1:A:316:LYS:HE3	1.75	0.43
1:A:148:ARG:HD3	1:A:148:ARG:HH11	1.65	0.43
1:A:277:GLU:OE2	1:A:342:TYR:OH	2.30	0.43
1:A:146:LYS:HE2	1:A:187:GLU:OE1	2.19	0.42
1:A:317:LYS:H	1:A:317:LYS:CE	2.31	0.42
1:A:146:LYS:HE3	2:A:394:HOH:O	2.19	0.42
1:A:89:ASP:OD1	1:A:91:ARG:CG	2.60	0.41
1:A:361:HIS:CG	1:A:362:ALA:N	2.85	0.41
1:A:59:ARG:O	1:A:63:LEU:HG	2.21	0.40

All (1) 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)
2:A:499:HOH:O	2:A:499:HOH:O[9_555]	1.04	1.16

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	360/363 (99%)	337 (94%)	18 (5%)	5 (1%)	9 5

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	350	ALA
1	A	351	ALA
1	A	347	GLN
1	A	345	SER
1	A	346	GLY

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	291/291 (100%)	261 (90%)	30 (10%)	7 4

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	13	LYS
1	A	38	SER
1	A	41	LYS
1	A	44	GLN
1	A	61	LEU
1	A	69	VAL
1	A	70	ASN
1	A	91	ARG
1	A	107	LYS
1	A	115	LEU
1	A	118	THR
1	A	123	THR
1	A	124	THR
1	A	173	TYR
1	A	207	LYS

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Mol	Chain	Res	Type
1	A	216	LEU
1	A	221	ILE
1	A	242	LYS
1	A	246	GLU
1	A	267	ILE
1	A	278	GLU
1	A	292	LEU
1	A	295	TRP
1	A	316	LYS
1	A	317	LYS
1	A	318	GLU
1	A	347	GLN
1	A	359	SER
1	A	363	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	70	ASN
1	A	80	HIS
1	A	119	ASN
1	A	166	ASN
1	A	178	GLN
1	A	245	HIS
1	A	306	GLN
1	A	324	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 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	362:ALA	C	363:TYR	N	2.13
1	A	350:ALA	C	351:ALA	N	1.71
1	A	344:PRO	C	345:SER	N	1.61

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.