



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 31, 2020 – 09:28 AM BST

PDB ID : 1DFK
Title : NUCLEOTIDE-FREE SCALLOP MYOSIN S1-NEAR RIGOR STATE
Authors : Houdusse, A.; Szent-Gyorgyi, A.G.; Cohen, C.
Deposited on : 1999-11-19
Resolution : 4.20 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
Xtriage (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) : 2.13

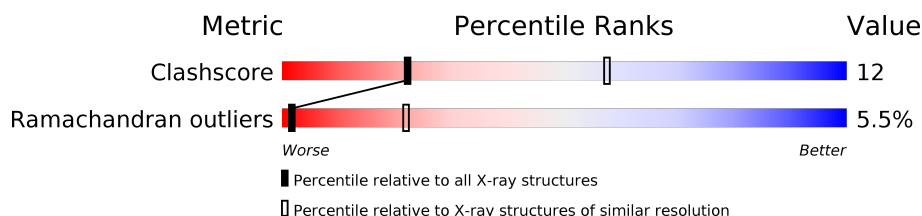
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.20 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	1044 (4.60-3.80)
Ramachandran outliers	138981	1000 (4.60-3.80)

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 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	830	
2	Y	139	
3	Z	152	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5032 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 MYOSIN HEAD.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	728	Total	C	N	O	0	0	0
			3597	2140	728	729			

- Molecule 2 is a protein called MYOSIN HEAD.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	Y	139	Total	C	N	O	0	0	0
			688	409	139	140			

- Molecule 3 is a protein called MYOSIN HEAD.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	Z	152	Total	C	N	O	0	0	0
			746	441	152	153			

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

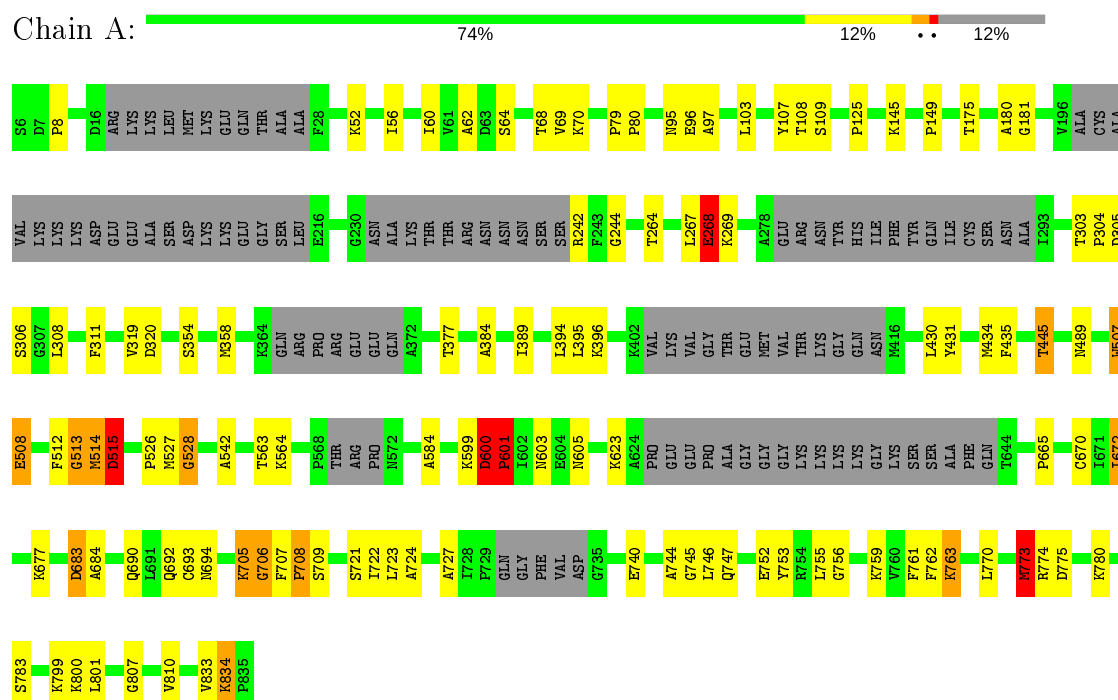
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	Z	1	Total	Ca	0	0
			1	1		

3 Residue-property plots

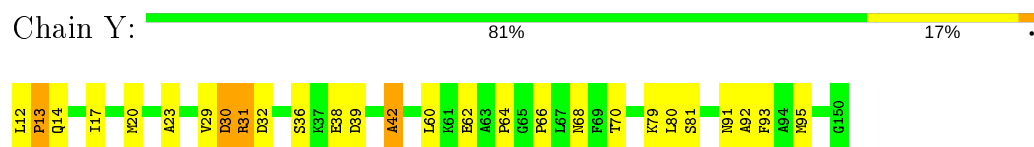
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

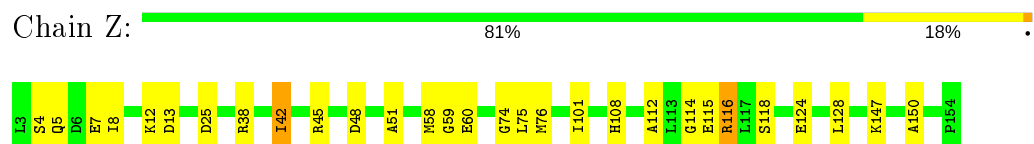
• Molecule 1: MYOSIN HEAD



• Molecule 2: MYOSIN HEAD



• Molecule 3: MYOSIN HEAD



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, α , β , γ	86.50 Å 52.10 Å 164.60 Å 90.00° 100.30° 90.00°	Depositor
Resolution (Å)	20.00 – 4.20	Depositor
% Data completeness (in resolution range)	95.0 (20.00-4.20)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.415 , 0.410	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5032	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	0.97	9/3587 (0.3%)	1.33	26/4978 (0.5%)
2	Y	0.42	0/687	0.80	2/954 (0.2%)
3	Z	0.58	1/745 (0.1%)	0.76	0/1031
All	All	0.86	10/5019 (0.2%)	1.20	28/6963 (0.4%)

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	8

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	268	GLU	C-N	-31.26	0.62	1.34
1	A	705	LYS	C-N	23.07	1.74	1.33
1	A	706	GLY	C-N	19.97	1.79	1.34
1	A	683	ASP	C-N	-18.55	0.91	1.34
3	Z	7	GLU	C-N	11.26	1.59	1.34
1	A	445	THR	C-N	-10.46	1.09	1.34
1	A	601	PRO	C-N	10.05	1.57	1.34
1	A	515	ASP	C-N	6.58	1.49	1.34
1	A	489	ASN	C-N	-6.11	1.20	1.34
1	A	709	SER	C-N	-5.03	1.22	1.34

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	515	ASP	O-C-N	-39.30	59.82	122.70
1	A	268	GLU	O-C-N	-35.48	65.94	122.70
1	A	268	GLU	C-N-CA	-24.70	59.95	121.70
1	A	268	GLU	CA-C-N	-24.51	63.29	117.20
1	A	515	ASP	CA-C-N	16.06	152.53	117.20
1	A	600	ASP	O-C-N	-12.07	98.17	121.10
1	A	683	ASP	CA-C-N	-11.54	91.81	117.20
1	A	773	MET	CA-C-N	-10.63	93.81	117.20
1	A	683	ASP	O-C-N	10.58	139.63	122.70
1	A	773	MET	O-C-N	9.98	138.66	122.70
1	A	706	GLY	O-C-N	8.75	136.70	122.70
1	A	709	SER	C-N-CA	7.21	139.73	121.70
1	A	706	GLY	CA-C-N	-7.11	101.56	117.20
1	A	600	ASP	CA-C-N	-6.66	98.46	117.10
1	A	601	PRO	C-N-CA	-6.09	106.47	121.70
2	Y	12	LEU	CB-CA-C	-6.09	98.63	110.20
1	A	708	PRO	N-CA-CB	5.68	110.12	103.30
2	Y	13	PRO	N-CA-CB	5.64	110.07	103.30
1	A	665	PRO	N-CA-CB	5.56	109.98	103.30
1	A	672	ILE	O-C-N	-5.55	110.56	121.10
1	A	8	PRO	N-CA-CB	5.41	109.79	103.30
1	A	125	PRO	N-CA-CB	5.39	109.77	103.30
1	A	79	PRO	N-CA-CB	5.31	109.67	103.30
1	A	80	PRO	N-CA-CB	5.25	109.60	103.30
1	A	683	ASP	C-N-CA	-5.24	108.61	121.70
1	A	677	LYS	N-CA-CB	5.22	119.99	110.60
1	A	677	LYS	O-C-N	5.21	131.04	122.70
1	A	599	LYS	N-CA-C	5.21	125.05	111.00

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	268	GLU	Mainchain
1	A	445	THR	Mainchain
1	A	515	ASP	Mainchain,Peptide
1	A	600	ASP	Mainchain
1	A	601	PRO	Mainchain
1	A	672	ILE	Mainchain
1	A	773	MET	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	3597	0	1592	58	0
2	Y	688	0	307	17	0
3	Z	746	0	340	11	0
4	Z	1	0	0	0	0
All	All	5032	0	2239	85	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 12.

All (85) 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:705:LYS:C	1:A:706:GLY:N	1.74	1.40
1:A:706:GLY:C	1:A:707:PHE:N	1.80	1.35
1:A:584:ALA:HB1	1:A:693:CYS:HA	1.37	1.07
1:A:770:LEU:O	1:A:774:ARG:CB	2.10	0.99
1:A:507:TRP:O	1:A:508:GLU:C	2.07	0.89
1:A:584:ALA:CB	1:A:693:CYS:HA	2.11	0.81
1:A:690:GLN:O	1:A:694:ASN:CB	2.34	0.76
2:Y:29:VAL:C	2:Y:31:ARG:H	1.95	0.69
1:A:706:GLY:CA	1:A:707:PHE:N	2.57	0.67
1:A:512:PHE:O	1:A:514:MET:N	2.32	0.63
1:A:683:ASP:O	1:A:684:ALA:C	2.33	0.61
1:A:706:GLY:C	1:A:707:PHE:CA	2.69	0.60
1:A:244:GLY:O	1:A:264:THR:HA	2.01	0.60
3:Z:58:MET:O	3:Z:60:GLU:N	2.32	0.60
2:Y:14:GLN:O	2:Y:17:ILE:N	2.34	0.59
1:A:740:GLU:O	1:A:744:ALA:HB2	2.03	0.59
2:Y:29:VAL:O	2:Y:31:ARG:N	2.36	0.58
1:A:507:TRP:O	1:A:508:GLU:O	2.23	0.56
1:A:773:MET:C	1:A:775:ASP:N	2.53	0.55
1:A:745:GLY:C	1:A:747:GLN:H	2.11	0.54
1:A:603:ASN:C	1:A:605:ASN:N	2.61	0.53
1:A:306:SER:C	1:A:308:LEU:H	2.12	0.53
1:A:319:VAL:O	1:A:320:ASP:C	2.47	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:807:GLY:O	2:Y:92:ALA:HB1	2.08	0.53
1:A:603:ASN:C	1:A:605:ASN:H	2.11	0.52
3:Z:147:LYS:O	3:Z:150:ALA:HB3	2.10	0.52
1:A:512:PHE:O	1:A:513:GLY:C	2.49	0.52
1:A:690:GLN:O	1:A:694:ASN:N	2.43	0.52
1:A:780:LYS:O	1:A:783:SER:N	2.43	0.51
3:Z:108:HIS:O	3:Z:112:ALA:HB3	2.11	0.51
1:A:430:LEU:O	1:A:434:MET:N	2.43	0.50
3:Z:114:GLY:O	3:Z:116:ARG:N	2.44	0.50
1:A:512:PHE:C	1:A:514:MET:N	2.62	0.50
1:A:745:GLY:O	1:A:747:GLN:N	2.45	0.49
1:A:512:PHE:C	1:A:514:MET:H	2.14	0.49
1:A:773:MET:C	1:A:775:ASP:H	2.16	0.49
2:Y:29:VAL:C	2:Y:31:ARG:N	2.64	0.49
1:A:95:ASN:O	1:A:97:ALA:N	2.46	0.49
1:A:584:ALA:HB1	1:A:693:CYS:CA	2.26	0.49
2:Y:20:MET:O	2:Y:23:ALA:HB3	2.13	0.48
1:A:180:ALA:HB1	1:A:670:CYS:CB	2.44	0.48
2:Y:38:GLU:O	2:Y:42:ALA:HB2	2.14	0.48
1:A:354:SER:O	1:A:358:MET:N	2.25	0.47
3:Z:48:ASP:O	3:Z:51:ALA:HB3	2.15	0.47
1:A:107:TYR:C	1:A:109:SER:H	2.18	0.47
1:A:384:ALA:HB1	1:A:389:ILE:O	2.15	0.47
2:Y:91:ASN:C	2:Y:93:PHE:N	2.68	0.47
1:A:527:MET:O	1:A:528:GLY:O	2.32	0.46
3:Z:12:LYS:O	3:Z:13:ASP:C	2.54	0.46
3:Z:38:ARG:HA	3:Z:42:ILE:O	2.15	0.46
1:A:56:ILE:O	1:A:68:THR:HA	2.16	0.46
1:A:833:VAL:O	1:A:834:LYS:C	2.53	0.45
1:A:431:TYR:O	1:A:435:PHE:N	2.29	0.45
2:Y:60:LEU:C	2:Y:62:GLU:H	2.20	0.45
1:A:303:THR:O	1:A:305:ASP:N	2.45	0.45
1:A:175:THR:O	1:A:670:CYS:N	2.38	0.45
3:Z:147:LYS:O	3:Z:150:ALA:N	2.49	0.45
1:A:756:GLY:HA3	1:A:759:LYS:O	2.16	0.45
2:Y:68:ASN:C	2:Y:70:THR:H	2.21	0.45
3:Z:74:GLY:C	3:Z:76:MET:H	2.21	0.44
2:Y:30:ASP:O	2:Y:32:ASP:N	2.50	0.44
2:Y:60:LEU:C	2:Y:62:GLU:N	2.69	0.44
1:A:394:LEU:O	1:A:396:LYS:N	2.50	0.44
2:Y:93:PHE:C	2:Y:95:MET:H	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:79:LYS:C	2:Y:81:SER:H	2.21	0.43
1:A:721:SER:C	1:A:723:LEU:H	2.20	0.43
1:A:762:PHE:O	1:A:763:LYS:O	2.37	0.43
2:Y:36:SER:O	2:Y:39:ASP:N	2.47	0.43
1:A:745:GLY:C	1:A:747:GLN:N	2.71	0.43
1:A:770:LEU:O	1:A:774:ARG:N	2.52	0.43
1:A:394:LEU:C	1:A:396:LYS:N	2.73	0.42
1:A:721:SER:O	1:A:723:LEU:N	2.51	0.42
2:Y:68:ASN:C	2:Y:70:THR:N	2.73	0.41
1:A:60:ILE:O	1:A:64:SER:HA	2.21	0.41
1:A:242:ARG:O	1:A:267:LEU:HA	2.20	0.41
1:A:762:PHE:C	1:A:763:LYS:O	2.58	0.41
1:A:799:LYS:C	1:A:801:LEU:H	2.24	0.41
1:A:705:LYS:CA	1:A:706:GLY:N	2.76	0.41
2:Y:93:PHE:C	2:Y:95:MET:N	2.74	0.41
3:Z:5:GLN:O	3:Z:8:ILE:N	2.53	0.41
1:A:563:THR:O	1:A:564:LYS:C	2.60	0.41
1:A:799:LYS:O	1:A:801:LEU:N	2.54	0.41
1:A:753:TYR:HA	1:A:761:PHE:O	2.22	0.40
3:Z:45:ARG:O	3:Z:48:ASP:N	2.54	0.40
1:A:69:VAL:O	1:A:70:LYS:C	2.58	0.40

There are no symmetry-related clashes.

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	708/830 (85%)	576 (81%)	95 (13%)	37 (5%)	2	22
2	Y	137/139 (99%)	96 (70%)	34 (25%)	7 (5%)	2	22
3	Z	150/152 (99%)	106 (71%)	33 (22%)	11 (7%)	1	16
All	All	995/1121 (89%)	778 (78%)	162 (16%)	55 (6%)	2	22

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	268	GLU
1	A	269	LYS
1	A	542	ALA
1	A	601	PRO
1	A	623	LYS
1	A	708	PRO
1	A	722	ILE
1	A	752	GLU
1	A	755	LEU
1	A	834	LYS
2	Y	31	ARG
3	Z	42	ILE
3	Z	75	LEU
3	Z	116	ARG
1	A	62	ALA
1	A	96	GLU
1	A	145	LYS
1	A	508	GLU
1	A	514	MET
1	A	528	GLY
1	A	746	LEU
1	A	763	LYS
2	Y	13	PRO
2	Y	30	ASP
2	Y	66	PRO
2	Y	80	LEU
3	Z	115	GLU
1	A	52	LYS
1	A	149	PRO
1	A	395	LEU
1	A	507	TRP
1	A	515	ASP
1	A	727	ALA
3	Z	25	ASP
3	Z	59	GLY
3	Z	124	GLU
1	A	311	PHE
1	A	377	THR
1	A	513	GLY
1	A	692	GLN
1	A	800	LYS
2	Y	42	ALA

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Mol	Chain	Res	Type
1	A	108	THR
1	A	526	PRO
3	Z	4	SER
3	Z	118	SER
1	A	103	LEU
3	Z	128	LEU
1	A	304	PRO
1	A	810	VAL
3	Z	101	ILE
1	A	181	GLY
1	A	600	ASP
2	Y	64	PRO
1	A	724	ALA

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	6

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	706:GLY	C	707:PHE	N	1.80
1	A	705:LYS	C	706:GLY	N	1.74
1	A	489:ASN	C	490:HIS	N	1.20
1	A	445:THR	C	446:LEU	N	1.10
1	A	683:ASP	C	684:ALA	N	0.91
1	A	268:GLU	C	269:LYS	N	0.62

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.