



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 02:36 am GMT

PDB ID : 1SCM
Title : STRUCTURE OF THE REGULATORY DOMAIN OF SCALLOP MYOSIN
AT 2.8 ANGSTROMS RESOLUTION
Authors : Cohen, C.; Xie, X.
Deposited on : 1994-01-06
Resolution : 2.80 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
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)	:	recalc28949

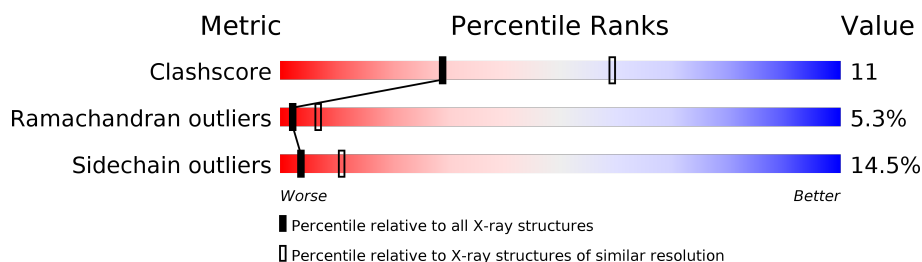
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)

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. 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	60	
2	B	145	
3	C	149	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2816 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 HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	60	Total	C	N	O	S	0	0	0
			529	350	102	76	1			

- Molecule 2 is a protein called MYOSIN REGULATORY LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	138	Total	C	N	O	S	0	0	0
			1107	701	176	221	9			

- Molecule 3 is a protein called MYOSIN ESSENTIAL LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	149	Total	C	N	O	S	0	0	0
			1178	743	188	240	7			

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

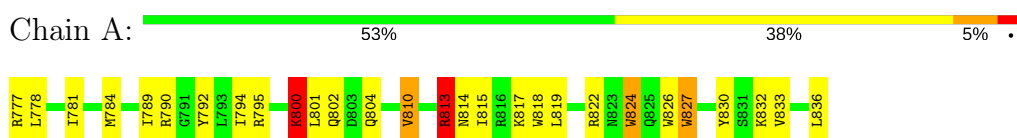
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		
4	C	1	Total	Ca	0	0
			1	1		

3 Residue-property plots [i](#)

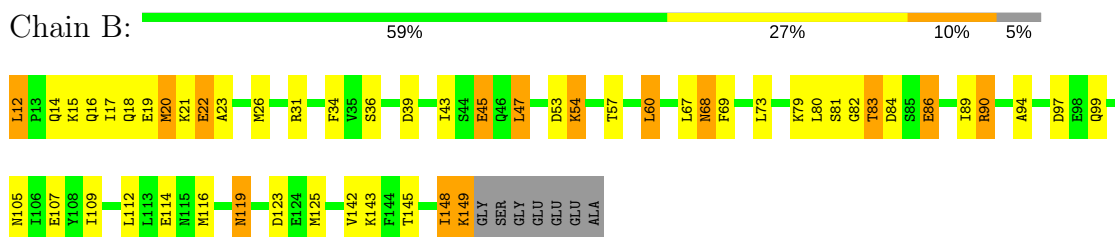
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

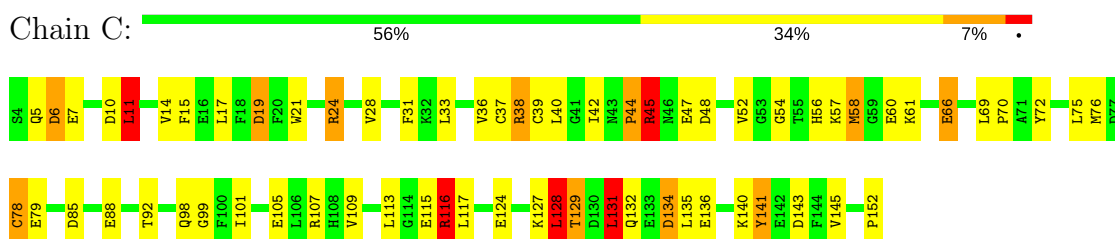
• Molecule 1: MYOSIN HEAVY CHAIN



• Molecule 2: MYOSIN REGULATORY LIGHT CHAIN



• Molecule 3: MYOSIN ESSENTIAL LIGHT CHAIN



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	52.50Å 87.00Å 55.50Å 90.00° 114.50° 90.00°	Depositor
Resolution (Å)	10.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.201 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2816	wwPDB-VP
Average B, all atoms (Å ²)	31.0	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	0.92	0/542	1.94	24/726 (3.3%)
2	B	0.81	0/1124	1.58	12/1502 (0.8%)
3	C	0.90	0/1200	1.86	27/1614 (1.7%)
All	All	0.87	0/2866	1.77	63/3842 (1.6%)

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
2	B	0	1
3	C	0	1
All	All	0	2

There are no bond length outliers.

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	128	LEU	CA-C-N	-15.54	83.01	117.20
1	A	790	ARG	NE-CZ-NH2	-10.90	114.85	120.30
1	A	818	TRP	CD1-CG-CD2	10.03	114.32	106.30
3	C	131	LEU	CA-C-N	-9.84	95.55	117.20
1	A	813	ARG	NE-CZ-NH1	9.41	125.00	120.30
3	C	129	THR	N-CA-C	-8.68	87.55	111.00
3	C	44	PRO	N-CA-C	8.40	133.94	112.10
3	C	21	TRP	CD1-CG-CD2	8.21	112.86	106.30
2	B	45	GLU	CA-CB-CG	8.19	131.42	113.40
1	A	818	TRP	CE2-CD2-CG	-7.96	100.93	107.30
3	C	21	TRP	CE2-CD2-CG	-7.81	101.06	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	826	TRP	CD1-CG-CD2	7.57	112.36	106.30
3	C	131	LEU	CA-C-O	7.45	135.74	120.10
1	A	826	TRP	CE2-CD2-CG	-7.39	101.38	107.30
1	A	822	ARG	NE-CZ-NH2	-7.34	116.63	120.30
1	A	827	TRP	CD1-CG-CD2	7.08	111.97	106.30
1	A	824	TRP	CD1-CG-CD2	7.08	111.97	106.30
1	A	827	TRP	CE2-CD2-CG	-7.02	101.68	107.30
2	B	148	ILE	CG1-CB-CG2	-6.90	96.22	111.40
2	B	20	MET	CA-CB-CG	6.88	125.00	113.30
2	B	31	ARG	NE-CZ-NH1	6.69	123.64	120.30
3	C	33	LEU	CA-CB-CG	6.59	130.46	115.30
3	C	141	TYR	CB-CG-CD2	-6.57	117.06	121.00
1	A	818	TRP	CG-CD1-NE1	-6.50	103.59	110.10
3	C	24	ARG	NE-CZ-NH1	6.49	123.55	120.30
3	C	79	GLU	CA-C-N	-6.44	103.04	117.20
1	A	777	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	A	824	TRP	CE2-CD2-CG	-6.29	102.27	107.30
2	B	20	MET	CG-SD-CE	6.25	110.20	100.20
3	C	98	GLN	N-CA-C	-6.24	94.15	111.00
2	B	81	SER	CA-C-N	-6.10	104.00	116.20
2	B	80	LEU	CA-CB-CG	6.06	129.24	115.30
1	A	826	TRP	CG-CD2-CE3	5.98	139.28	133.90
1	A	826	TRP	CB-CG-CD1	-5.82	119.43	127.00
3	C	116	ARG	CA-C-N	-5.82	104.39	117.20
3	C	88	GLU	CA-CB-CG	5.81	126.17	113.40
3	C	44	PRO	C-N-CA	5.80	136.20	121.70
1	A	813	ARG	NE-CZ-NH2	-5.77	117.42	120.30
2	B	31	ARG	NE-CZ-NH2	-5.77	117.42	120.30
3	C	107	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	A	810	VAL	CG1-CB-CG2	-5.74	101.72	110.90
3	C	44	PRO	CA-N-CD	-5.62	103.63	111.50
2	B	39	ASP	CB-CA-C	-5.62	99.16	110.40
3	C	6	ASP	N-CA-C	-5.57	95.97	111.00
3	C	128	LEU	O-C-N	5.55	131.58	122.70
3	C	38	ARG	CA-CB-CG	-5.45	101.42	113.40
2	B	14	GLN	CB-CG-CD	5.44	125.74	111.60
2	B	125	MET	CG-SD-CE	-5.37	91.61	100.20
1	A	777	ARG	CB-CG-CD	-5.31	97.79	111.60
3	C	78	CYS	CA-CB-SG	5.24	123.43	114.00
1	A	790	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	A	818	TRP	CG-CD2-CE3	5.17	138.55	133.90
3	C	79	GLU	CA-CB-CG	-5.15	102.06	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	57	LYS	CA-C-N	-5.12	105.92	117.20
3	C	24	ARG	CA-CB-CG	5.11	124.64	113.40
1	A	800	LYS	CA-CB-CG	5.09	124.60	113.40
3	C	11	LEU	CB-CG-CD1	-5.09	102.35	111.00
3	C	19	ASP	CB-CG-OD1	5.08	122.87	118.30
3	C	115	GLU	N-CA-CB	-5.07	101.48	110.60
1	A	795	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	A	784	MET	CG-SD-CE	-5.01	92.19	100.20
1	A	800	LYS	CB-CG-CD	5.01	124.62	111.60
2	B	22	GLU	CA-CB-CG	5.00	124.41	113.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	12	LEU	Peptide
3	C	128	LEU	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	529	0	577	18	0
2	B	1107	0	1092	23	0
3	C	1178	0	1104	32	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
All	All	2816	0	2773	61	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 11.

All (61) 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)
3:C:127:LYS:HG3	3:C:128:LEU:H	1.34	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:127:LYS:HG3	3:C:128:LEU:N	2.04	0.72
1:A:810:VAL:HG22	1:A:813:ARG:NH2	2.05	0.72
2:B:145:THR:O	2:B:148:ILE:HG22	1.93	0.68
1:A:789:ILE:HG21	3:C:117:LEU:HD21	1.78	0.66
2:B:90:ARG:HD3	2:B:142:VAL:HG13	1.82	0.62
3:C:124:GLU:O	3:C:127:LYS:HG2	2.00	0.62
3:C:7:GLU:HB3	3:C:10:ASP:HB2	1.81	0.62
2:B:68:ASN:HD22	2:B:69:PHE:N	1.98	0.61
3:C:42:ILE:HD12	3:C:72:TYR:CE1	2.37	0.60
2:B:114:GLU:O	2:B:119:ASN:HB3	2.02	0.59
1:A:824:TRP:CE3	1:A:827:TRP:HB2	2.38	0.59
3:C:141:TYR:O	3:C:145:VAL:HG23	2.04	0.58
1:A:794:ILE:HG22	3:C:39:CYS:SG	2.44	0.58
3:C:42:ILE:HD12	3:C:72:TYR:HE1	1.70	0.56
3:C:31:PHE:CD2	3:C:58:MET:HG2	2.41	0.56
1:A:810:VAL:HG22	1:A:813:ARG:HH22	1.70	0.56
3:C:42:ILE:HD13	3:C:76:MET:HA	1.89	0.55
3:C:19:ASP:HA	3:C:28:VAL:HG12	1.88	0.55
3:C:14:VAL:HG12	3:C:36:VAL:HG13	1.89	0.54
2:B:43:ILE:HG13	2:B:47:LEU:HD22	1.89	0.53
2:B:94:ALA:HA	2:B:97:ASP:HB3	1.93	0.51
1:A:792:TYR:CZ	3:C:152:PRO:HA	2.46	0.50
2:B:19:GLU:O	2:B:22:GLU:HB3	2.11	0.50
3:C:15:PHE:CE1	3:C:28:VAL:HG13	2.46	0.50
2:B:109:ILE:HA	2:B:112:LEU:HD12	1.94	0.50
2:B:145:THR:O	2:B:149:LYS:HB2	2.12	0.49
1:A:830:TYR:HE1	2:B:23:ALA:HB2	1.76	0.49
3:C:127:LYS:CG	3:C:128:LEU:N	2.73	0.47
3:C:11:LEU:HA	3:C:40:LEU:HD11	1.97	0.47
1:A:817:LYS:HG2	2:B:83:THR:HG23	1.97	0.46
1:A:836:LEU:HD12	2:B:26:MET:HE1	1.96	0.46
2:B:148:ILE:HD13	2:B:148:ILE:HG21	1.63	0.46
1:A:781:ILE:HD12	3:C:85:ASP:HB3	1.98	0.46
1:A:815:ILE:HG12	2:B:148:ILE:HD12	1.98	0.46
1:A:830:TYR:OH	2:B:19:GLU:HG2	2.16	0.45
3:C:38:ARG:HH12	3:C:45:ARG:NH2	2.15	0.45
1:A:833:VAL:HG13	2:B:26:MET:HE2	1.97	0.45
2:B:68:ASN:HD22	2:B:69:PHE:H	1.65	0.45
3:C:37:CYS:SG	3:C:75:LEU:CD1	3.06	0.45
3:C:19:ASP:CA	3:C:28:VAL:HG12	2.47	0.44
1:A:800:LYS:O	1:A:804:GLN:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:66:GLU:O	3:C:70:PRO:HD3	2.17	0.44
2:B:57:THR:O	2:B:60:LEU:HD12	2.18	0.43
3:C:42:ILE:HD11	3:C:76:MET:HG3	2.01	0.43
3:C:128:LEU:HD12	3:C:128:LEU:HA	1.94	0.43
3:C:47:GLU:OE2	3:C:78:CYS:HB2	2.19	0.43
1:A:814:ASN:HD21	2:B:84:ASP:HB2	1.84	0.42
3:C:140:LYS:HE3	3:C:140:LYS:HB3	1.81	0.42
1:A:794:ILE:CG2	3:C:39:CYS:SG	3.07	0.42
3:C:105:GLU:O	3:C:109:VAL:HG13	2.18	0.42
1:A:824:TRP:HE3	1:A:827:TRP:HB2	1.83	0.42
1:A:813:ARG:HG3	1:A:813:ARG:HH11	1.85	0.42
3:C:135:LEU:HA	3:C:135:LEU:HD12	1.81	0.42
2:B:12:LEU:O	2:B:17:ILE:HD13	2.20	0.41
2:B:15:LYS:HG3	2:B:16:GLN:H	1.85	0.41
2:B:21:LYS:HB3	2:B:69:PHE:CZ	2.55	0.41
2:B:34:PHE:HA	2:B:67:LEU:O	2.20	0.41
3:C:38:ARG:HH12	3:C:45:ARG:HH21	1.67	0.41
3:C:6:ASP:O	3:C:7:GLU:HG3	2.21	0.41
3:C:101:ILE:HG22	3:C:141:TYR:HB3	2.01	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	58/60 (97%)	54 (93%)	4 (7%)	0	100	100
2	B	136/145 (94%)	117 (86%)	12 (9%)	7 (5%)	2	7
3	C	147/149 (99%)	118 (80%)	18 (12%)	11 (8%)	1	2
All	All	341/354 (96%)	289 (85%)	34 (10%)	18 (5%)	2	7

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	83	THR
3	C	5	GLN
3	C	44	PRO
3	C	56	HIS
3	C	92	THR
2	B	79	LYS
3	C	54	GLY
3	C	131	LEU
3	C	52	VAL
3	C	99	GLY
3	C	116	ARG
3	C	134	ASP
2	B	86	GLU
2	B	89	ILE
2	B	90	ARG
3	C	45	ARG
2	B	54	LYS
2	B	82	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	56/56 (100%)	49 (88%)	7 (12%)	5	16
2	B	122/126 (97%)	103 (84%)	19 (16%)	3	9
3	C	125/125 (100%)	107 (86%)	18 (14%)	4	11
All	All	303/307 (99%)	259 (86%)	44 (14%)	4	11

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	778	LEU
1	A	800	LYS
1	A	801	LEU
1	A	802	GLN
1	A	813	ARG

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Mol	Chain	Res	Type
1	A	819	LEU
1	A	832	LYS
2	B	18	GLN
2	B	20	MET
2	B	36	SER
2	B	45	GLU
2	B	47	LEU
2	B	53	ASP
2	B	54	LYS
2	B	60	LEU
2	B	68	ASN
2	B	73	LEU
2	B	86	GLU
2	B	99	GLN
2	B	105	ASN
2	B	107	GLU
2	B	116	MET
2	B	119	ASN
2	B	123	ASP
2	B	143	LYS
2	B	149	LYS
3	C	11	LEU
3	C	17	LEU
3	C	24	ARG
3	C	45	ARG
3	C	48	ASP
3	C	58	MET
3	C	60	GLU
3	C	61	LYS
3	C	66	GLU
3	C	69	LEU
3	C	113	LEU
3	C	116	ARG
3	C	129	THR
3	C	131	LEU
3	C	132	GLN
3	C	134	ASP
3	C	136	GLU
3	C	143	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	814	ASN
2	B	68	ASN
2	B	115	ASN
3	C	5	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](#)

Of 2 ligands modelled in this entry, 2 are 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 [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.