



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:07 PM UTC

PDB ID : 1SCM / pdb_00001scm
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

<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

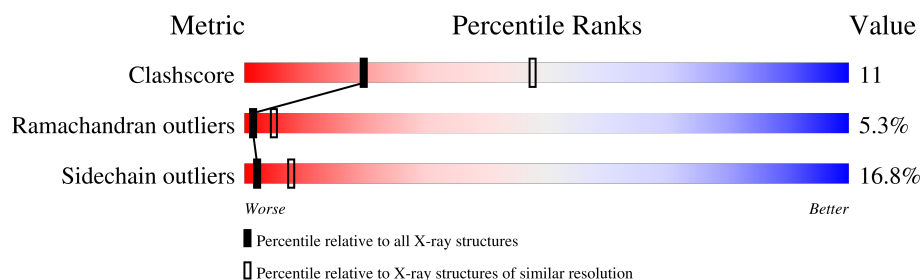
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (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 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	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 (CCD ID: 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

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.

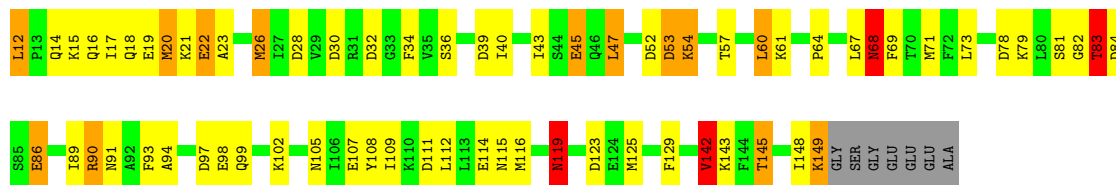
• Molecule 1: MYOSIN HEAVY CHAIN

Chain A: 



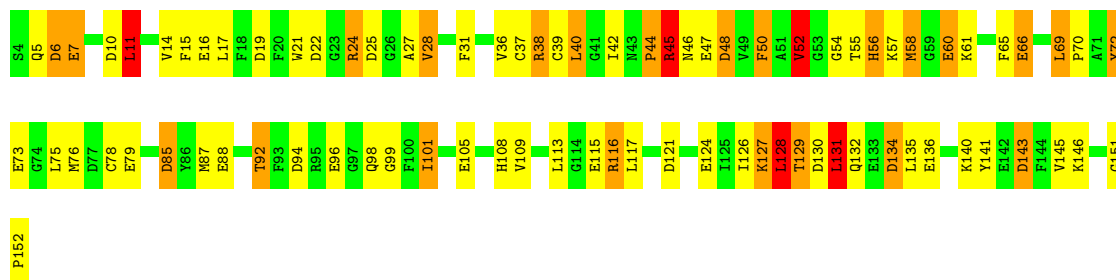
• Molecule 2: MYOSIN REGULATORY LIGHT CHAIN

Chain B: 



• Molecule 3: MYOSIN ESSENTIAL LIGHT CHAIN

Chain C: 



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	1.13	2/542 (0.4%)	2.06	19/726 (2.6%)
2	B	0.98	0/1124	2.04	41/1502 (2.7%)
3	C	1.10	3/1200 (0.2%)	2.28	58/1614 (3.6%)
All	All	1.06	5/2866 (0.2%)	2.15	118/3842 (3.1%)

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	788	HIS	CD2-NE2	-6.03	1.31	1.37
3	C	56	HIS	CD2-NE2	-5.48	1.31	1.37
1	A	788	HIS	CG-ND1	-5.35	1.32	1.38
3	C	108	HIS	CD2-NE2	-5.25	1.32	1.37
3	C	126	ILE	CA-C	5.03	1.59	1.52

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	6	ASP	N-CA-C	-13.56	95.97	111.03
3	C	50	PHE	CA-CB-CG	-11.82	101.98	113.80
3	C	129	THR	N-CA-C	-10.91	87.55	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	130	ASP	CA-CB-CG	10.69	123.29	112.60
3	C	131	LEU	CA-C-O	10.65	135.74	120.51
3	C	44	PRO	N-CA-C	10.42	133.94	112.47
3	C	22	ASP	CA-CB-CG	9.47	122.07	112.60
2	B	91	ASN	CA-CB-CG	9.38	121.97	112.60
3	C	98	GLN	N-CA-C	-9.36	94.15	109.40
2	B	93	PHE	CA-CB-CG	9.12	122.92	113.80
3	C	46	ASN	CA-CB-CG	9.04	121.64	112.60
3	C	128	LEU	O-C-N	8.79	131.58	123.50
2	B	45	GLU	CA-CB-CG	8.66	131.42	114.10
3	C	108	HIS	CA-CB-CG	-8.64	105.16	113.80
3	C	57	LYS	N-CA-C	8.61	123.47	108.75
2	B	91	ASN	N-CA-C	-8.60	101.84	111.82
3	C	108	HIS	CA-C-O	-8.46	111.49	120.55
3	C	11	LEU	N-CA-C	-8.22	102.40	111.36
2	B	45	GLU	N-CA-C	-7.99	102.65	111.36
3	C	108	HIS	N-CA-C	-7.99	101.66	111.40
3	C	60	GLU	N-CA-C	7.92	119.60	110.97
2	B	145	THR	CA-C-O	-7.78	112.83	121.00
2	B	14	GLN	CB-CG-CD	7.73	125.74	112.60
3	C	44	PRO	CA-C-N	7.68	136.20	121.54
3	C	44	PRO	C-N-CA	7.68	136.20	121.54
2	B	32	ASP	CA-CB-CG	7.67	120.27	112.60
3	C	96	GLU	N-CA-C	7.54	122.31	113.18
2	B	108	TYR	N-CA-C	-7.45	102.77	111.03
2	B	28	ASP	N-CA-C	-7.27	98.90	109.59
3	C	48	ASP	CA-CB-CG	7.25	119.86	112.60
2	B	78	ASP	N-CA-C	-7.20	101.69	111.55
1	A	825	GLN	N-CA-C	7.18	119.97	111.71
3	C	56	HIS	CB-CG-CD2	-7.14	121.92	131.20
3	C	146	LYS	N-CA-C	6.94	119.44	111.11
2	B	14	GLN	OE1-CD-NE2	-6.91	115.69	122.60
3	C	121	ASP	CA-CB-CG	6.80	119.40	112.60
2	B	30	ASP	N-CA-C	6.79	121.23	113.15
3	C	101	ILE	N-CA-C	-6.71	98.45	108.12
3	C	85	ASP	CA-CB-CG	6.66	119.26	112.60
3	C	143	ASP	CA-CB-CG	-6.57	106.03	112.60
2	B	98	GLU	CB-CG-CD	6.40	123.49	112.60
3	C	38	ARG	CA-CB-CG	-6.34	101.42	114.10
2	B	52	ASP	N-CA-C	6.33	124.29	110.80
2	B	39	ASP	CB-CA-C	-6.30	99.16	110.70
3	C	73	GLU	N-CA-C	6.30	118.96	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	68	ASN	OD1-CG-ND2	-6.29	116.31	122.60
3	C	55	THR	N-CA-C	6.28	119.88	112.72
1	A	794	ILE	CB-CA-C	-6.27	103.84	112.24
3	C	72	TYR	N-CA-C	-6.22	104.42	111.14
3	C	79	GLU	CA-C-O	6.22	126.83	120.24
1	A	801	LEU	CA-C-O	6.17	126.48	119.27
2	B	61	LYS	N-CA-C	-6.13	106.06	112.93
2	B	28	ASP	CA-CB-CG	6.12	118.72	112.60
2	B	81	SER	O-C-N	6.07	130.90	123.01
3	C	88	GLU	CA-CB-CG	6.04	126.17	114.10
3	C	79	GLU	CA-CB-CG	-6.02	102.06	114.10
3	C	44	PRO	CA-N-CD	-5.98	103.63	112.00
2	B	39	ASP	N-CA-CB	5.94	119.05	110.20
3	C	129	THR	O-C-N	-5.92	114.71	122.59
1	A	782	ILE	O-C-N	-5.90	116.11	121.89
1	A	777	ARG	CB-CG-CD	-5.88	97.79	111.30
3	C	65	PHE	CA-CB-CG	-5.85	107.95	113.80
3	C	7	GLU	CB-CG-CD	5.84	122.53	112.60
1	A	800	LYS	CB-CG-CD	5.79	124.62	111.30
3	C	45	ARG	N-CA-C	5.76	123.06	110.80
3	C	27	ALA	CA-C-O	-5.75	113.70	120.60
3	C	69	LEU	CA-C-O	-5.74	113.05	118.33
2	B	64	PRO	N-CA-C	-5.69	102.16	111.21
3	C	25	ASP	CA-CB-CG	5.66	118.26	112.60
3	C	130	ASP	O-C-N	5.60	130.04	122.59
3	C	56	HIS	CA-CB-CG	5.57	119.37	113.80
2	B	115	ASN	OD1-CG-ND2	-5.56	117.04	122.60
2	B	53	ASP	N-CA-C	-5.52	99.05	110.80
2	B	93	PHE	N-CA-C	-5.50	107.11	113.88
3	C	115	GLU	N-CA-CB	-5.50	101.48	110.11
2	B	142	VAL	N-CA-C	-5.49	105.02	111.00
2	B	30	ASP	CA-CB-CG	5.48	118.08	112.60
3	C	79	GLU	O-C-N	5.48	129.68	123.27
2	B	14	GLN	CG-CD-NE2	5.47	124.60	116.40
2	B	83	THR	N-CA-C	5.47	122.44	110.80
2	B	20	MET	CA-CB-CG	5.45	125.00	114.10
1	A	788	HIS	CB-CG-CD2	-5.42	124.15	131.20
3	C	94	ASP	CA-CB-CG	5.42	118.02	112.60
2	B	111	ASP	CA-CB-CG	5.41	118.01	112.60
3	C	151	GLY	O-C-N	-5.40	116.37	121.77
3	C	87	MET	CA-C-O	-5.40	113.42	119.79
3	C	46	ASN	N-CA-C	-5.39	104.81	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	826	TRP	CG-CD2-CE3	5.38	139.28	133.90
3	C	128	LEU	N-CA-C	-5.37	97.88	107.28
3	C	92	THR	CA-CB-OG1	-5.37	101.55	109.60
2	B	26	MET	CA-C-N	5.35	127.50	120.60
2	B	26	MET	C-N-CA	5.35	127.50	120.60
1	A	786	GLN	CG-CD-NE2	5.33	124.39	116.40
2	B	83	THR	CA-CB-OG1	-5.30	101.65	109.60
2	B	115	ASN	CA-CB-CG	5.30	117.90	112.60
3	C	115	GLU	CB-CG-CD	-5.29	103.60	112.60
1	A	786	GLN	OE1-CD-NE2	-5.29	117.31	122.60
2	B	102	LYS	N-CA-C	5.28	117.78	109.39
3	C	24	ARG	CA-CB-CG	5.27	124.64	114.10
2	B	119	ASN	CA-CB-CG	5.27	117.87	112.60
2	B	39	ASP	CA-CB-CG	5.27	117.87	112.60
1	A	814	ASN	OD1-CG-ND2	-5.25	117.35	122.60
1	A	800	LYS	CA-CB-CG	5.25	124.60	114.10
1	A	809	SER	CA-C-O	-5.24	114.87	120.42
2	B	40	ILE	N-CA-C	-5.24	105.28	110.62
1	A	818	TRP	CE2-CD2-CG	-5.23	100.93	107.20
1	A	793	LEU	CA-C-N	5.19	128.86	120.55
1	A	793	LEU	C-N-CA	5.19	128.86	120.55
2	B	22	GLU	CA-CB-CG	5.15	124.41	114.10
1	A	785	PHE	N-CA-C	-5.14	105.59	111.14
3	C	21	TRP	CE2-CD2-CG	-5.12	101.06	107.20
3	C	126	ILE	N-CA-CB	-5.11	102.81	111.23
3	C	143	ASP	O-C-N	5.09	127.31	122.07
1	A	818	TRP	CG-CD1-NE1	-5.08	103.59	110.20
3	C	52	VAL	N-CA-CB	-5.03	102.93	111.23
2	B	22	GLU	N-CA-C	-5.02	105.72	111.14
1	A	818	TRP	CD1-CG-CD2	5.01	114.32	106.30
3	C	56	HIS	CB-CG-ND1	5.01	130.21	122.70

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	17	0
2	B	1107	0	1092	24	0
3	C	1178	0	1104	34	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
All	All	2816	0	2773	64	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 (64) 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
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
1:A:836:LEU:HD12	2:B:26:MET:HE1	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:125:MET:HE3	2:B:129:PHE:HE1	1.75	0.51
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:125:MET:HE3	2:B:129:PHE:CE1	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:76:MET:HB3	3:C:76:MET:HE2	1.57	0.48
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
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
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
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:794:ILE:CG2	3:C:39:CYS:SG	3.07	0.42
1:A:814:ASN:HD21	2:B:84:ASP:HB2	1.84	0.42
3:C:140:LYS:HB3	3:C:140:LYS:HE3	1.81	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:HH11	1:A:813:ARG:HG3	1.85	0.42
3:C:135:LEU:HD12	3:C:135:LEU:HA	1.81	0.42
2:B:12:LEU:O	2:B:17:ILE:HD13	2.20	0.41
3:C:50:PHE:C	3:C:52:VAL:H	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:101:ILE:HG22	3:C:141:TYR:HB3	2.01	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	58/60 (97%)	54 (93%)	4 (7%)	0	100	100
2	B	136/145 (94%)	117 (86%)	12 (9%)	7 (5%)	1	5
3	C	147/149 (99%)	118 (80%)	18 (12%)	11 (8%)	1	2
All	All	341/354 (96%)	289 (85%)	34 (10%)	18 (5%)	1	5

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

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Mol	Chain	Res	Type
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%)	4	15
2	B	122/126 (97%)	101 (83%)	21 (17%)	2	7
3	C	125/125 (100%)	102 (82%)	23 (18%)	1	6
All	All	303/307 (99%)	252 (83%)	51 (17%)	2	8

All (51) 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
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	71	MET
2	B	73	LEU
2	B	86	GLU
2	B	99	GLN

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Mol	Chain	Res	Type
2	B	105	ASN
2	B	107	GLU
2	B	116	MET
2	B	119	ASN
2	B	123	ASP
2	B	142	VAL
2	B	143	LYS
2	B	149	LYS
3	C	11	LEU
3	C	16	GLU
3	C	17	LEU
3	C	24	ARG
3	C	28	VAL
3	C	40	LEU
3	C	45	ARG
3	C	48	ASP
3	C	52	VAL
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	127	LYS
3	C	129	THR
3	C	131	LEU
3	C	132	GLN
3	C	134	ASP
3	C	136	GLU
3	C	143	ASP

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

Mol	Chain	Res	Type
1	A	804	GLN
2	B	68	ASN
3	C	5	GLN
3	C	46	ASN

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](#)

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.