

# Full wwPDB NMR Structure Validation Report (i)

### Mar 11, 2021 - 02:09 am GMT

PDB ID	:	6ZBI
Title	:	Ternary complex of Calmodulin bound to 2 molecules of NHE1
Authors	:	Prestel, A.; Kragelund, B.B.; Pedersen, E.S.; Pedersen, S.F.; Sjoegaard-Frich,
		L.M.
Deposited on	:	2020-06-08

This is a Full wwPDB NMR 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/NMRValidationReportHelp with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

$\operatorname{MolProbity}$	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. $(2010)$
${ m ShiftChecker}$	:	2.17.1
Ideal geometry (proteins)	:	Engh & Huber $(2001)$
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.17.1

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $SOLUTION\ NMR$ 

The overall completeness of chemical shifts assignment is 84%.

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 $(\#Entries)$	(# Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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 <=5%

Mol	Chain	Length	Quality of chain	
1	А	148	78%	10% 11%
2	В	36	67%	31%
2	С	36	58% 8%	33%



# 2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 6 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues						
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model			
1	A:7-A:73, C:824-C:847 (91)	0.39	6			
2	A:85-A:148, B:622-B:646	0.43	12			
	(89)					

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 4 clusters and 2 single-model clusters were found.

Cluster number	Models
1	9, 13, 14, 16, 17, 20
2	1, 2, 5, 10, 11
3	6, 12, 18, 19
4	3, 4, 8
Single-model clusters	7; 15



# 3 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3537 atoms, of which 1749 are hydrogens and 0 are deuteriums.

• Molecule 1 is a protein called Calmodulin-1.

Mol	Chain	Residues			Atom	IS			Trace
1	Λ	140	Total	С	Η	Ν	0	$\mathbf{S}$	0
	A	140	2261	714	1095	188	255	9	0

• Molecule 2 is a protein called Sodium/hydrogen exchanger 1.

Mol	Chain	Residues		At	oms			Trace
0	В	26	Total	С	Η	Ν	Ο	0
	2 D	50	636	187	327	65	57	0
0	C	26	Total	С	Η	Ν	Ο	0
	U	- 50	636	187	327	65	57	0

• Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms
3	А	4	Total Ca
		-	4 4



# 4 Residue-property plots (i)

### 4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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 outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

 Chain A:
 78%
 10%
 11%

 Image: Imag

### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

### 4.2.1 Score per residue for model 1

• Molecule 1: Calmodulin-1

• Molecule 1: Calmodulin-1





### V142 K148

428458

• Molecule 2: Sodium/hydrogen exchanger 1

Chain B:	67%	•	31%
4622 1623 1623 1623 8649 1650 1650 1650 1655 1655 1655 1655 1655	<b>1967</b>		
• Molecule 2: Sod	ium/hydrogen exchanger	: 1	
Chain C:	61%	6%	33%
4822 1823 1823 1825 1825 1831 1851 1851 1852	L854 V 855 A 855 D857 D857		
4.2.2 Score pe	r residue for model 2		
• Molecule 1: Cal	modulin-1		
Chain A:	76%		12% 11%
A1 14 15 15 15 12 12 12 12 12 12 12 12 12 12 12 12 12	N35 N35 N56 N56 N56 N50 N56 N57 N75 N75 N77 N77 N77 N77 N77 N77 N77	179 180 881 883 883 883 883 883 884 884 884 898 199 1116	V121 D131 Y138 V142 K148
• Molecule 2: Sod	ium/hydrogen exchanger	: 1	
Chain B:	64%	6%	31%
<b>A622</b> 1638 1637 1638 1647 1653 1655 1655 1653 1653 1653	V655 A656 D657		
• Molecule 2: Sod	ium/hydrogen exchanger	: 1	
Chain C:	58%	6% ·	33%
A822 L823 L823 1834 1834 L835 S848 Y849 N850 R851 R851	1283 1865 1865 1887 1887		
4.2.3 Score pe	r residue for model 3		
• Molecule 1: Cal	modulin-1		
Chain A:	76%		12% • 11%

F65 P66 K77 K77 K77 D78 D80 D80 D80 D80 B82 E833 E833 E833

> D W I D E DATA BANK

NGO GG1 TG2

- Molecule 2: Sodium/hydrogen exchanger 1 Chain B: ' 31% 67% • Molecule 2: Sodium/hydrogen exchanger 1 Chain C: 56% 8% 33% Y849 N850 N851 H852 H853 T853 V855 V855 4.2.4Score per residue for model 4 • Molecule 1: Calmodulin-1 Chain A: 74% 14% 11%P64 F65 P66 E67 F66 R74 K75 M76 K77 D78 D78 D78 D80 S81 E82 E83 E83 E83 A1 03 15 15 15 15 • Molecule 2: Sodium/hydrogen exchanger 1 Chain B: 58% 11% 31% S648 Y649 N650 N651 H652 T652 T652 V655 A656 A656 • Molecule 2: Sodium/hydrogen exchanger 1 Chain C: 58% 6% 33% . Score per residue for model 5 4.2.5• Molecule 1: Calmodulin-1 Chain A: 72% 17% 11% D78 T79 D80 S81 E82
- 01<mark>35</mark> K148



• Molecule 2: Sodium/hydrogen exchanger 1 Chain B: 61% 31% 8% H652 T653 L654 V655 A656 A656 • Molecule 2: Sodium/hydrogen exchanger 1 Chain C: 61% 6% 33% Y849 N850 R851 H852 T853 T853 L854 V855 A856 4.2.6Score per residue for model 6 (medoid) • Molecule 1: Calmodulin-1 Chain A: 76% 12% 11% . K75 K77 K77 T79 T79 D80 S81 E82 E83 E83 • Molecule 2: Sodium/hydrogen exchanger 1 Chain B: 67% 31% • Molecule 2: Sodium/hydrogen exchanger 1 Chain C: 61% 6% 33% Score per residue for model 7 4.2.7• Molecule 1: Calmodulin-1



• Molecule 2: Sodium/hydrogen exchanger 1



Chain B:	64%	•• 31	%
A622 L635 M638 R647	Y649 Y649 H6551 T6552 T6554 V6555 A655 A655		
• Molecul	e 2: Sodium/hydrogen exchanger 1		
Chain C:	61% 69	% 33%	
4822 1323 1831 1834	8848 1851 1855 1855 1855 1855 1855 1855		
4.2.8 S	core per residue for model 8		
• Molecul	e 1: Calmodulin-1		
Chain A:	76%	11%	• 11%
4 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2	118 128 128 128 128 158 158 158 158 158 158 158 158 158 15	E83 E84 D93 G98 T99 D129	1130 1131 1131 1135 1135 1135 1138 1138 1138
• Molecul	e 2: Sodium/hydrogen exchanger 1		
Chain B:	64%	6% 31	%
A622 N638 L639 R647 S648	Y649 N650 R651 T653 T653 T655 A656 A656		
• Molecul	e 2: Sodium/hydrogen exchanger 1		
Chain C:	61% 69	% 33%	
4822 1823 1831 1834	Y 848 Y 849 Y 8551 A 8555 V 8555 V 8555 V 8555 V 8555		
4.2.9 S	core per residue for model 9		
• Molecul	e 1: Calmodulin-1		
Chain A:	76%	11%	• 11%
A1 02 15 15 15	112 118 118 118 128 128 128 158 168 168 168 168 168 168 168 178 178 178 178 178 178 178 178 178 17	822 833 100 100 100 100 100 100 100 100 100 1	4135 Y142 V142 K148

• Molecule 2: Sodium/hydrogen exchanger 1

Chain B: 67% · 31%



### A622 N638 N658 N650 N650 N650 N650 N650 N655 L654 L654 L655 L655 L655 D657

• Molecule 2: Sodium/hydrogen exchanger 1

Chain C: 61% 6% 33%

### 4.2.10 Score per residue for model 10

• Molecule 1: Calmodulin-1



 $\bullet$  Molecule 2: Sodium/hydrogen exchanger 1

Chain B:	69%	31%
622 647 644 655 655 655 655 655 655 655 655		

• Molecule 2: Sodium/hydrogen exchanger 1

Chair	1	C:						_						58%	8%	33%	
A822 L823 1831		1834 1835	<b>0</b> 00	20402	Y849	N850	R851	H852	T853	L854	V855	A856	D857				

### 4.2.11 Score per residue for model 11

• Molecule 1: Calmodulin-1



• Molecule 2: Sodium/hydrogen exchanger 1

Chain B:	67%	•	31%
4622 N638 N650 N650 N650 N650 R651 H655 V655 D657 D657			



• Molecule 2: Sodium/hydrogen exchanger 1

Chain C:	56%	11%	33%
A822 L823 1831 1834 L835 L835	1842 8448 17849 17850 18850 18852 18852 18852 188555 18855 18855 18855 18855 188555 18855 18855 18855 18855 18855		

### 4.2.12 Score per residue for model 12

• Molecule 1: Calmodulin-1

Chain A:	78%		9% •	11%
A 1 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2	F68 K75 M76 M76 M77 179 B81 B83 B83 B83	N97 199 1130 1131 1130 1131	K148	
• Molecule 2: Sodium/hydro	gen exchanger 1			
Chain B:	51%	8%	31%	
4622 NG38 L639 L639 R643 N654 N654 N655 T653 T655 T655 T655 T655 A655 A655				
• Molecule 2: Sodium/hydro	gen exchanger 1			
Chain C: 58	%	8%	33%	
4822 1823 1823 1834 1834 1855 1855 1855 1855 1855 1855 1855 185				
4.2.13 Score per residue	e for model 13			
• Molecule 1: Calmodulin-1				
Chain A:	79%		9%	11%
A1 02 03 03 03 03 04 05 05 05 05 05 05 05 05 05 05 05 05 05	M72 473 473 877 777 777 777 777 881 882 883 883 884	N97 <b>G98</b> L1112 L1116 Q135	M1 44	
• Molecule 2: Sodium/hydro	gen exchanger 1			
Chain B:	67%	·	31%	
4622 1635 1647 1649 10650 10650 10652 1654 1655 1655 1655 1655 1655 1655				

 $\bullet$  Molecule 2: Sodium/hydrogen exchanger 1



A622 L623 L623 N638 N647 Y649 N650 N650 N650 L654 L655 L655 L655 L655 A656

• Molecule 2: Sodium/hydrogen exchanger 1

Chain C:	58%	8%	33%
A822 L823 S824 K825 L835 L835 L835 L835 S848 Y849 Y849 N850 R851 R851	T3853 12854 V8655 A8665 D857		
4.2.14 Score p	per residue for model	14	
• Molecule 1: Cal	lmodulin-1		
Chain A:	76%		13% 11%
022 719 024 025 025 025 025 025 025 025 025 025 025	116 116 116 116 116 116 116 116 116 116	M76 1779 1779 1779 1779 1779 1779 1784 1794 1794 1794 1794 1794 1794 1794 179	116 116 1116 1131 116 1131 116 116 116 1
• Molecule 2: Soc	lium/hydrogen exchange:	r 1	
Chain B:	64%	6%	31%
A6 22 L6 35 N6 38 N6 47 S6 48 N6 50 N6 50 N6 50 N6 51 T6 53 T76 52	1655 4656 1657		
• Molecule 2: Soc	dium/hydrogen exchange:	r 1	
Chain C:	64%	•	33%
A822 L823 L823 1831 N850 N850 N855 1855 L855 V855 V855	A866 D857		
	-		
4.2.15 Score p	per residue for model	15	
• Molecule 1: Cal	lmodulin-1		
Chain A:	73%		15% • 11%
12 12 12 12 12 12 12 12 12 12 12 12 12 1	128 M36 M51 M51 M51 M60 M60 M60 M60 M60 M60 M60 M60 M60 M60	M72 A73 K75 K75 K75 M76 T79 B81 B82 E83 E83	84 100 100 100 100 100 100 100 111 1117 1117
0135 K148			
• Molecule 2: Soc	dium/hydrogen exchange:	r 1	
Chain B:	64%	6%	31%

L D W I D E

ww

Chain C:	56%	11%	33%
4822 1831 1834 1834 1834 1835 1834 1835 1885 1885 1885 1885	1853 V855 A856 D857		
4.2.16 Score per	residue for mode	l 16	
• Molecule 1: Calmo	dulin-1		
Chain A:	76%		12% 11%
A1 11 11 11 11 11 11 11 11 11 11 11 11 1	126 M36 D56 M60 M60 F68 F68 K74 M76	K/7 179 188 183 183 183 183 183 183 183 193 193 193 193 193 193	Y99 D129 D131 0131 1130 V135 V142 V142 V142
• Molecule 2: Sodium	n/hydrogen exchang	ger 1	
Chain B:	69%		31%
4622 R647 S649 V650 N650 R651 H655 H655 L654 V655 A656 V655 A656			
• Molecule 2: Sodium	${ m n/hydrogen}~{ m exchang}$	ger 1	
Chain C:	58%	8%	33%
4822 1881 1881 1884 1884 1884 1885 1885 1885	V855 8866 D8667		
4.2.17 Score per	residue for mode	l 17	
• Molecule 1: Calmo	dulin-1		
Chain A:	76%		12% • 11%
41 11 11 11 11 11 11 11 11 11 11 11 11 1	V35 N36 L48 L48 G50 G61 160 R74 K75 M76	K77 179 179 188 183 188 188 188 188 199 199 199 199	1116 1130 1130 1130 1130 1130 1130 1130
• Molecule 2: Sodium	${ m n/hydrogen}$ exchang	er 1	
Chain B:	67%	•	31%
4622 N638 N638 N647 N651 N651 N655 T653 T655 T655 N655 N655 N655 N655			
• Molecule 2: Sodium	n/hydrogen exchang	ger 1	
Chain C:	61%	6%	33%
		PROTEIN DATA BANK	

### A822 L823 L823 L835 L835 N850 N850 N850 L855 L855 L855 L855 L855 D857 D857

### 4.2.18 Score per residue for model 18

• Molecule 1: Calmodulin-1

Chain A:	74%		14% 119	6
A1 11 11 11 11 11 11 12 12 12 12 12 12 12	659 661 762 661 762 766 776 776 777 779 880 882 882	B83 B84 B93 M109 M109 B1100 B100 B10 B1	1110 1111 1126 1130 1131	4138 1138 1142 1143 1143 1143
K 148				
• Molecule 2: Sodium	/hydrogen exchanger 1			
Chain B:	61%	8%	31%	_
4622 1635 1638 1646 1644 1653 1653 1653 1653 1653 1653 1653	A656 D657			
• Molecule 2: Sodium	/hydrogen exchanger 1			
Chain C:	64%	·	33%	_
4822 1823 1885 1885 1885 1885 1885 1885 1885 188				
4.2.19 Score per r	esidue for model 19			
• Molecule 1: Calmod	ulin-1			
Chain A:	78%		10% • 11	%
A1 03 154 155 156 156 122 126 128 128 128 128 128 128 128 128 128 128	N60 661 762 773 773 773 775 777 779 779 779 881 882 882	E83 E84 N97 Y108 V108	L116 Q135 M145 K148	
• Molecule 2: Sodium	/hydrogen exchanger 1			
Chain B:	64%	6%	31%	
4622 1634 1634 1639 1653 1655 1655 1655 1655 1655 1655	29 <u>90</u>			
• Molecule 2: Sodium	/hydrogen exchanger 1			
Chain C:	58%	8%	33%	_
	W C	PDB TEIN DATA BANK		

# 

### 4.2.20 Score per residue for model 20

• Molecule 1: Calmodulin-1

Chain A:	71%	16	5% • 11%	-
M1 115 115 115 115 115 115 115 115 115 1	061 1162 1162 1163 1163 165 166 168 175 178 178 178 178 178 178	881 882 883 884 892 698 698	Y99 H107 V108 N111 L116	V121 D122 E123 D129 D129 1130
0131 0135 0135 0136 0146 0148				
• Molecule 2: Sodium/hyd	rogen exchanger 1			
Chain B:	64%	6%	31%	_
4622 1634 1634 1634 1634 1635 1655 1655 1655 1655 1655 1655 1655				
• Molecule 2: Sodium/hyd	rogen exchanger 1			
Chain C:	61%	6%	33%	_

GLOBAL-STATISTICS INFOmissingINFO

S848 Y849 N850 R851 H852 H852 L854 V855 A856 A856 D857

A822 L823



# 5 Model quality (i)

## 5.1 Standard geometry (i)

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

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	А	1027	966	967	$13\pm2$
2	В	215	239	236	1±1
2	С	213	234	234	2±1
3	А	4	0	0	8±2
All	All	29180	28780	28740	273

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 5.

All unique clashes are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	$Clash(\lambda)$	Distance(Å)	Models	
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total
1:A:116:LEU:HD23	1:A:121:VAL:HG22	0.72	1.62	20	5
1:A:18:LEU:HG	2:C:831:ILE:HD11	0.67	1.65	5	6
1:A:97:ASN:OD1	3:A:203:CA:CA	0.66	1.73	4	20
1:A:60:ASN:OD1	3:A:202:CA:CA	0.66	1.72	16	19
1:A:135:GLN:O	3:A:204:CA:CA	0.65	1.74	3	16
1:A:62:THR:O	3:A:202:CA:CA	0.64	1.75	11	19
1:A:55:VAL:HG11	1:A:71:MET:SD	0.64	2.32	19	1
1:A:26:THR:O	3:A:201:CA:CA	0.64	1.75	18	20
1:A:99:TYR:O	3:A:203:CA:CA	0.64	1.75	7	20

Continued on next page...



	1 5			Models		
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total	
1:A:93:ASP:OD1	3:A:203:CA:CA	0.63	1.76	7	8	
1:A:20:ASP:OD1	3:A:201:CA:CA	0.62	1.77	14	9	
1:A:129:ASP:OD1	3:A:204:CA:CA	0.62	1.77	16	5	
1:A:24:ASP:OD1	3:A:201:CA:CA	0.62	1.77	7	7	
1:A:56:ASP:OD1	3:A:202:CA:CA	0.61	1.78	15	9	
1:A:18:LEU:HB3	2:C:831:ILE:HD11	0.61	1.70	15	7	
1:A:91:VAL:HG21	2:B:623:LEU:HD22	0.61	1.73	15	3	
1:A:137:ASN:OD1	3:A:204:CA:CA	0.60	1.78	10	1	
1:A:36:MET:HG2	2:C:835:LEU:HD13	0.60	1.72	1	7	
1:A:18:LEU:HD13	2:C:831:ILE:HD11	0.58	1.75	10	4	
2:B:639:LEU:HD21	2:B:643:ARG:HE	0.57	1.59	12	1	
1:A:27:ILE:HD12	1:A:68:PHE:CE1	0.56	2.34	1	3	
1:A:19:PHE:HA	1:A:35:VAL:HG21	0.56	1.75	20	13	
1:A:63:ILE:HG21	1:A:68:PHE:CE1	0.56	2.36	14	3	
1:A:116:LEU:HD13	2:B:639:LEU:HD11	0.53	1.80	2	1	
1:A:36:MET:SD	2:C:835:LEU:HD13	0.50	2.47	15	5	
1:A:32:LEU:HD22	1:A:48:LEU:HD11	0.49	1.85	17	1	
1:A:44:THR:HG23	1:A:47:GLU:H	0.49	1.66	8	1	
1:A:109:MET:CE	2:B:635:LEU:HD12	0.49	2.37	7	1	
1:A:92:PHE:CD2	1:A:108:VAL:HG21	0.48	2.44	6	3	
1:A:117:THR:HG23	1:A:120:GLU:H	0.48	1.69	5	2	
1:A:12:PHE:CD2	1:A:69:LEU:HD12	0.48	2.44	1	1	
1:A:105:LEU:HD23	1:A:121:VAL:HG13	0.48	1.86	11	1	
1:A:142:VAL:O	1:A:146:THR:HG23	0.47	2.09	17	1	
1:A:138:TYR:O	1:A:142:VAL:HG23	0.46	2.10	9	6	
1:A:63:ILE:HG21	1:A:68:PHE:CD1	0.46	2.45	9	2	
1:A:36:MET:HG3	2:C:835:LEU:HD13	0.46	1.86	12	1	
1:A:91:VAL:HG21	2:B:623:LEU:HD11	0.45	1.88	5	1	
1:A:107:HIS:CE1	1:A:111:ASN:HD21	0.45	2.29	20	1	
1:A:144:MET:SD	2:B:635:LEU:HD21	0.45	2.52	18	2	
1:A:145:MET:O	2:B:634:ILE:HD13	0.45	2.12	20	2	
1:A:52:ILE:HG23	1:A:63:ILE:HD11	0.45	1.89	20	1	
1:A:123:GLU:OE1	2:B:646:LEU:HD13	0.45	2.12	20	1	
1:A:12:PHE:CE2	1:A:69:LEU:HD12	0.44	2.48	1	1	
1:A:109:MET:HG2	1:A:116:LEU:HD22	0.44	1.88	6	1	
1:A:51:MET:HG2	2:C:842:THR:HG21	0.44	1.90	15	4	
1:A:18:LEU:HD23	2:C:831:ILE:HD11	0.44	1.89	9	1	
1:A:88:ALA:HA	2:B:623:LEU:HD11	0.43	1.89	1	1	
1:A:51:MET:O	1:A:55:VAL:HG23	0.43	2.12	3	2	
2:B:639:LEU:O	2:B:639:LEU:HD13	0.43	2.13	19	1	
1:A:72:MET:CE	2:C:834:ILE:CG2	0.43	2.96	19	4	

Continued from previous page...

Continued on next page...



Atom 1	Atom 2	$Clash(\lambda)$	Distance(Å)	Models	
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total
2:C:834:ILE:CG2	2:C:835:LEU:N	0.42	2.82	4	2
1:A:130:ILE:HD11	1:A:143:GLN:HG2	0.42	1.90	17	1
1:A:65:PHE:N	1:A:66:PRO:HD2	0.42	2.30	5	6
1:A:32:LEU:O	1:A:32:LEU:HD23	0.41	2.16	17	1
1:A:39:LEU:HD11	2:C:831:ILE:CG2	0.41	2.46	1	1
1:A:65:PHE:N	1:A:66:PRO:CD	0.41	2.84	20	2
1:A:27:ILE:HD12	1:A:68:PHE:CD1	0.41	2.51	12	1
1:A:109:MET:CE	2:B:635:LEU:HD23	0.40	2.45	5	1
1:A:13:LYS:HA	1:A:16:PHE:CD1	0.40	2.51	1	1
1:A:55:VAL:HG12	1:A:55:VAL:O	0.40	2.16	2	1
1:A:112:LEU:HD22	2:B:632:ARG:HE	0.40	1.76	4	1

Continued from previous page...

### 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 PDB entries followed by that with respect to all NMR entries. 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	А	130/148~(88%)	$130\pm0$ (100 $\pm0\%$ )	0±0 (0±0%)	0±0 (0±0%)	100	100
2	В	24/36~(67%)	$24\pm0~(100\pm0\%)$	0±0 (0±0%)	0±0 (0±0%)	100	100
2	С	24/36~(67%)	$24\pm0$ (100 $\pm0\%$ )	0±0 (0±0%)	0±0 (0±0%)	100	100
All	All	3560/4400~(81%)	3560~(100%)	0 (0%)	0  (0%)	100	100

There are no Ramachandran outliers.

### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. 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	А	110/126~(87%)	$106 \pm 1 \ (96 \pm 1\%)$	$4\pm1~(4\pm1\%)$	36 84	

Continued on next page...



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
2	В	24/34~(71%)	$23 \pm 1 \ (96 \pm 3\%)$	$1 \pm 1 (4 \pm 3\%)$	36	84	
2	С	24/34~(71%)	$23 \pm 1 \ (98 \pm 3\%)$	$1 \pm 1 \ (2 \pm 3\%)$	53	92	
All	All	3160/3880~(81%)	3047~(96%)	113 (4%)	38	86	

Continued from previous page...

All 30 unique residues with a non-rotameric side chain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	А	131	ASP	17
1	А	58	ASP	13
2	В	638	ASN	13
1	А	116	LEU	10
2	С	834	ILE	8
1	А	18	LEU	5
1	А	68	PHE	5
1	А	22	ASP	4
1	А	12	PHE	4
1	А	109	MET	3
1	А	72	MET	2
2	С	835	LEU	2
1	А	36	MET	2
2	В	646	LEU	2
2	В	635	LEU	2
1	А	56	ASP	2
1	А	129	ASP	2
1	А	126	ARG	2
1	А	48	LEU	2
1	А	16	PHE	2
1	А	145	MET	2
1	А	69	LEU	1
1	А	52	ILE	1
2	В	639	LEU	1
1	А	51	MET	1
1	А	112	LEU	1
2	С	825	LYS	1
1	А	94	LYS	1
1	А	28	THR	1
1	А	111	ASN	1



### 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 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

### 5.7 Other polymers (i)

There are no such molecules in this entry.

### 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry. CHEMICAL-SHIFTS INFOmissingINFO

